

Supplementary Information

Data mining, dashboards and statistics: a powerful framework for the chemical design of molecular nanomagnets

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Supplementary Section 1. Construction of the dataset

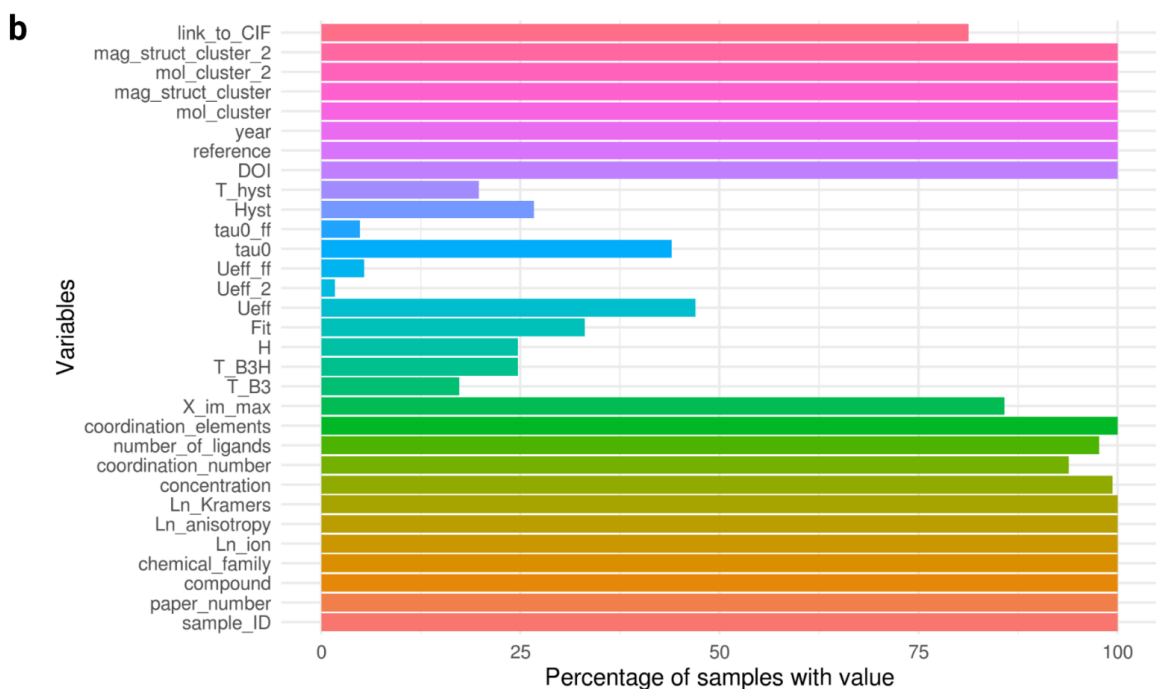
Data extraction was restricted to variables that can be systematically extracted from articles included in the present study. Our objectives for the data analysis were twofold: the correlation between different variables of the same (physical or chemical) category and the correlation between two variables from different (chemical and physical) categories. In the first case, the goal is to determine whether the variables are closely correlated with each other, and thus to simplify our analysis and to avoid false correlations. In the second case, the goal is to determine which chemical variables are proven to be the most influential on the physical performance.

For physical variables, we focus on the magnetic hysteresis and the behaviour of the out-of-phase component of the ac susceptibility. These two kinds of experimental observations are the most basic experimental tell-tale signs for SIM behaviour. For both, we extract from the articles qualitative and quantitative information. For ac susceptibility, we extract as qualitative information whether the out-of-phase component of the ac susceptibility χ'' vs the temperature has a maximum when there is no external dc magnetic field, or whether this maximum is absent but there is a frequency-dependent behaviour of χ'' with the temperature. As quantitative information, we extract the temperature of said χ'' vs T maximum. If the maximum of the out-of-phase component of the ac susceptibility appears in the presence of an external dc magnetic field, we extract the temperature at which the said maximum value appears and the applied external field. From reported magnetisation vs the magnetic field experiments, we extract as qualitative information the presence of full hysteresis (with remnant magnetisation and/or a coercive field), or at least a pinched hysteresis, and as quantitative information the maximum hysteresis temperature reported. In addition, a series of variables from the more extended theoretical analysis of the experimental data, namely the effective energy barrier U_{eff} and the relaxation time τ_0 , as well as relevant information on what kind of fit gave rise to these parameters are also included.

In the case of the chemical variables, the information we collected and analysed is as follows: (a) the chemical family of the complex; (b) the lanthanide (Ln) ion; (c) whether the Ln ion is oblate, prolate or isotropic; (d) whether the Ln ion is Kramers or not; (e) the concentration of the sample (if the diamagnetic dilution is studied); (f) the coordination number of the Ln ion; (g) the number of coordinated ligands; (h) the coordination elements.

A full list of the variables, including the number of data points and the percentage of samples with valid values for each variable in the dataset, can be found in Supplementary Fig. 1.

a			
Chemical Variables	N	Physical Variables	N
Chemical Family	1405	χ_{\max}'' : Presence of maximum in $\chi''(T)$	1206
Ln ion	1405	T_{B3} : Temperature of χ_{\max}'' at zero-field	244
Ln anisotropy	1405	T_{B3H} : Temperature of χ_{\max}'' at field H	347
Ln Kramers	1405	H : External Applied Magnetic Field	347
Concentration	1396	Fit : U_{eff} fitted by T_{B3} or Argand	465
Coordination Number	1319	U_{eff} : Effective barrier with Orbach process	660
Number of Ligands	1373	$U_{\text{eff}2}$: U_{eff} for a second relaxation process	24
Coordination Elements	1405	$U_{\text{eff,ff}}$: U_{eff} for all processes (full fit)	76
		τ_0 : Attempt time with Orbach process	618
		$\tau_{0,\text{ff}}$: Attempt time with all relaxation processes	68
		Hyst : Presence of pinched or full hysteresis	375
		T_{Hyst} : Maximum hysteresis temperature	278



Supplementary Figure 1.1 | Chemical and physical variables included in the dataset. a, Correspondence between variables and symbols and number (N) of samples in the dataset containing that information. **b,** Percentage of samples containing valid values for each variable.

Let us start by defining the chemical variables and explaining the different values they can take. When appropriate a numerical labelling equivalence for each value is given in square brackets, this is used in some of the statistical plots in later sections.

-The parameter “Chemical family” is categorical and takes one of the following 9 values for each sample: {LnPc₂ [1]; polyoxometalate [2]; Schiff base [3]; metallocene [4]; diketonate [5]; radical [6]; TM near Ln [7]; mixed ligands [8]; other families [9]}. Details on this classification are given in Supplementary Section 2.

-The parameter “Ln ion” is categorical and takes one of the following 10 values for each sample: {Pr³⁺ [1]; Nd³⁺ [2]; Sm³⁺ [3]; Gd³⁺ [4]; Tb³⁺ [5]; Dy³⁺ [6]; Ho³⁺ [7]; Er³⁺ [8]; Tm³⁺ [9]; Yb³⁺ [10]}.

-The parameter “Ln anisotropy” is categorical and takes one of the following 3 values for each sample: {prolate [0]; oblate [1]; isotropic [2]}. This is determined directly by the Ln ion.

-The parameter “Ln Kramers” is categorical and takes one of the following 2 values for each sample: {non Kramers [0]; Kramers [1]}. Like the anisotropy, this is determined directly by the Ln ion.

-The parameter “concentration” takes the percentage value, e.g. concentration=1 is read as 1% concentration of the magnetic lanthanide ion in a diamagnetic matrix where 99% of the molecules are *e.g.* the Y³⁺ analog.

-The parameter “Coordination Number” (or CN) is an integer number between 2 and 9. Note that, for LnPc₂ we assigned CN = 8, as corresponding to the 8 N donor atoms; and for metallocenes we assigned CN = 2, assuming that the electron density is delocalized within each aromatic ring.

-The parameter “Number of ligands” is an integer number between 2 and 9, corresponding to the total number of ligands contributing donor atoms. The absolute number of ligands is registered, not the number of chemically different ligands: N identical ligands count as N.

-The parameter “Coordination Elements” is categorical and takes one of the following 5 values for each sample: {Oxygen [1]; Nitrogen [2]; Oxygen+Nitrogen [3]; Carbon [4]; Others [5]}. Any combination of oxygens and nitrogens is counted as “Oxygen+Nitrogen”, and complexes with coordination elements different from O, N or C in the coordination sphere of lanthanide ions are in the category of “Others”.

Let us continue by defining the physical variables.

-The parameter labelled as χ''_{\max} (in plots), or $\chi_{\text{im},\max}$ (in data table), takes one of these possible values:

·[0]: Freq-independent χ'' (neither $T_{B3} > 2$ K reported, nor frequency-dependence in χ'' vs T),

- [1]: Freq-dependent χ'' (no $T_{B3} > 2$ K, but frequency-dependence in χ'' vs T measured),
- [2]: $T_{B3} > 2$ K, and
- [3]: Not Measured (no available data to assign the sample into one of the previous three categories).

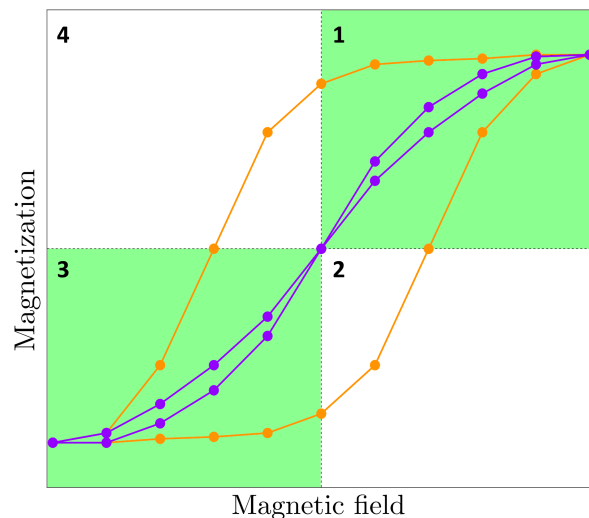
$-T_{B3}$ (T_{B3H}) is the temperature at which one finds the maximum value of χ'' vs T at 10^3 Hz, in absence (in presence) of an external magnetic field; H is the magnetic field, if present. It can be understood as the maximum temperature for which the system maintains short-term (millisecond) magnetic memory. For articles that provide χ'' vs T with a curve for each different frequency, we simply chose the curve corresponding to the frequency 10^3 Hz (or the closest one) and registered the temperature for the maximum χ'' , or the absence of a maximum. However, if the articles represent χ'' vs frequency as isothermal curves for each different temperature, the same information is accessible indirectly by reading the points in the graph vertically at the abscissa value corresponding to the frequency 10^3 Hz and checking in consecutive temperature curves whether χ'' values present a non-monotonic evolution with respect to temperature, and therefore a maximum.

-“Fit” registers whether the parameters to determine U_{eff} and τ_0 were obtained from $\chi''(T)$ maxima at different frequencies or from an Argand plot.

$-U_{\text{eff}}$, $U_{\text{eff},2}$, $U_{\text{eff},\text{ff}}$ are the effective energy barriers and τ_0 , $\tau_{0,\text{ff}}$ are the attempt times, which means the pre-exponential factors. The values of the effective energy barrier U_{eff} and of the attempt time τ_0 are recorded if they are determined from a fit considering a single Orbach process. In the cases where a second Orbach process is considered, we register (besides U_{eff} , τ_0 for the first process) its effective energy barrier $U_{\text{eff},2}$. If a more complete model for relaxation is employed including an Orbach process as well as the Raman process, Quantum Tunneling of the Magnetization and/or a direct process, we consider this a “full fit”(in short: ff), and record the value of the effective energy barrier $U_{\text{eff},\text{ff}}$ and the attempt time or pre-exponential factor $\tau_{0,\text{ff}}$.

-The parameter labelled as “*Hyst*” takes one of the four values as follows:

- [0]: No hysteresis above 2 K reported,
- [1]: Pinched Hysteresis (magnetic hysteresis above 2 K reported, but no magnetic coercivity field or remnant magnetisation can be determined; see Supplementary Fig. 1.2),
- [2]: Full Hysteresis (magnetic hysteresis above 2 K reported, and additionally either magnetic coercive field or remnant magnetisation can be determined; see Supplementary Fig. 1.2),
- [3]: Not Measured (no available data to assign the sample into one of the previous three categories).



Supplementary Figure 1.2 | Full vs pinched hysteresis. Full hysteresis curves (orange) present at least one point either in quadrants 2,4 (*i.e.* different signs for Magnetic field and Magnetization) or in the x and/or y axes. Pinched hysteresis curves (violet) present points only in quadrants 1,3 (*i.e.* same signs for H and M) and, sometimes, also at the origin of coordinates.

-The related parameter “ T_{hyst} ” takes the highest temperature value at which hysteresis is reported. In contrast with T_{B3} , this quantifies the temperature up to which the system maintains long-term magnetic memory.

One of the main problems for the data extraction during the construction of the dataset was that different criteria are chosen by different groups to characterize the hysteresis. For example, the hysteresis is measured only at 2 K in many studies, resulting in an overrepresentation of $T_{\text{hyst}} = 2$ in the dataset; while in many other cases the hysteresis is measured up to the highest possible temperature. Therefore, the very same compound could then present different T_{hyst} depending on an arbitrary choice by the researchers, decreasing the quality of the dataset. Another difficulty is that the information of the applied magnetic field sweep rate which directly affects T_{hyst} is missing in some articles. In addition, in some articles, not only a full hysteresis, presenting coercive field and magnetic remanence, is measured up to a certain temperature but also a pinched hysteresis is measured up to a higher temperature. This introduces some noise in the dataset, but is less problematic since both cases are going to be registered as a SIM with good properties.

Supplementary Section 2. Classification in chemical families

Lanthanides are a group of f -block elements with atomic number ranging from 57 (lanthanum) to 71 (lutetium). Most of the Ln elements exhibit the oxidation state of +3. Our dataset only includes the trivalent Ln^{3+} (Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm and Yb) ions containing

complexes. Ln ions possess large coordination numbers (CNs) due to their large ionic radii. The geometrical arrangement around these trivalent ions basically depends on the steric properties of the coordinated ligands; thus a suitable design of the ligand molecules leads to an easy tuning of the CNs. In particular, CNs between 2 and 12 are documented for Ln ions. Note that in this work we consider one rigid aromatic ring as equivalent to a contribution to CN/ring = 1 when it is of the cyclopentadienyl/cyclooctatetraenyl kind, whereas we consider a contribution of CN/ring = 4 when it is of the phthalocyaninato kind. In the low CN cases, the coordination ligands are usually bulky ligands, e.g. bis(trimethylsilyl) amine gives CN = 3; whereas cyclopentadienyl ligands need to be smartly substituted to achieve the same steric impediment. In contrast, in the case of complexes with high CN, the ligands are usually small bidentate ligands, such as nitrate and/or macrocyclic ligands. In the present work, we found that the most frequent are CN = 8 and CN = 9. This coincides with what is known for Ln ions, namely, Ln ions tend to spontaneously favour these CNs, typically with distorted square antiprismatic coordination (CN = 8) or distorted tricapped trigonal prism coordination (CN = 9).

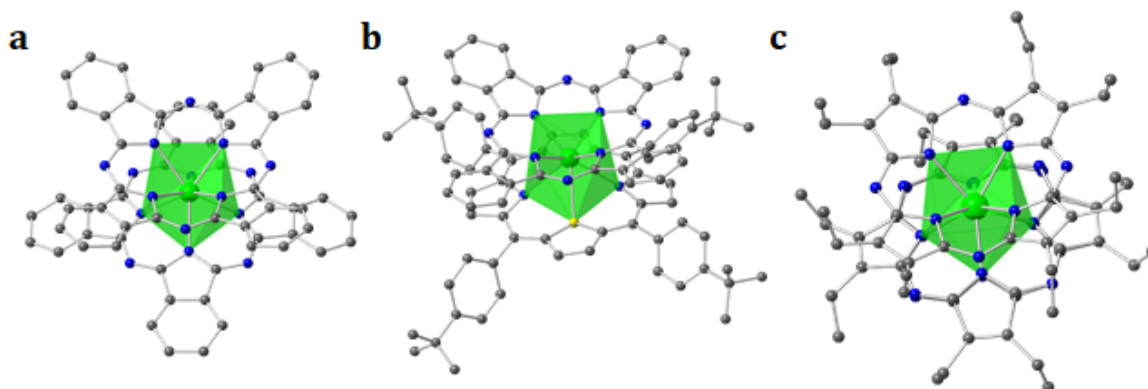
Ln-based SIMs are interesting because the $4f$ electrons are less exposed to ligand field effects and exhibit larger spin-orbital coupling if compared with the d -shell. The first Ln-based mononuclear single molecule magnets (SMMs) were generated by Ishikawa and co-workers in 2003 using two macrocyclic ligands to sandwich the Ln^{3+} ion in a double-decker fashion.¹ They can also be prepared by using a range of acyclic ligands, such as polyoxometalates (POMs),^{2–4} Schiff bases,^{5,6} radicals,^{7–15} and ketones.^{16–18} Between 2003 and 2019, several hundreds of articles referring to Ln-based SIMs have been published. Among them, the vast majority focused on the chemical approaches in designing lanthanide-based SIMs with superior properties. A fundamental key parameter of the magnetic properties of SIMs is the molecular symmetry which can be controlled by: (a) the ligand design and modification, (b) the substitution of the coordination elements as a means to alter electrostatic potential and/or Ln to coordination atom bond lengths, and (c) the peripheral ligand functionalization/substitution. Here, we classify the collected complexes into 9 categories according to the type of coordination ligands or the chemical strategy used for the design of the magnetic complex. These 9 categories (Chemical Family) are listed below and will be briefly described in this section.

- 1) LnPc_2 family
- 2) POM family
- 3) Schiff Base family
- 4) Metallocene family
- 5) Diketonate family
- 6) Radical family
- 7) TM near Ln family
- 8) Mixed ligands family
- 9) Other families

2.1. LnPc₂ family

The first category is constituted by “double-decker complexes” related to the classical LnPc₂ family, namely, the Ln ion in the complex is octa-coordinated by nitrogen atoms from two Pc (or their related functionalized complexes, or porphyrin-like, or even tetraaza[14]annulenes) ligands. As we will see below, this criterion has priority over the presence of a spin $S = 1/2$ (radical ligand, in this case corresponding to oxidized or reduced Pc ligands) and also over the presence of diamagnetic transition metal ions in the vicinity (in this case often corresponding to multiple deckers which coordinate Cd³⁺). In both cases, these complexes are classified as LnPc₂ family. Complexes composed of phthalocyanine ligands or porphyrins with nitrogen-based donating atoms have shown very important roles in Ln-based SIMs. There are several reasons for choosing phthalocyanines and porphyrins for SIM design: a) these tetrapyrrole macrocyclic ligands containing four isoindole or pyrrole nitrogen atoms have the ability to strongly coordinate to Ln ions; b) special features such as intramolecular π - π stacking interaction and the intrinsic nature of their macrocyclic rotation;¹⁹ and c) their structural characteristics of those sandwich-type complexes since the ligand field constructed by this type of ligands with a C₄-symmetric axis (pseudo- D_{4d} symmetry) is very important for the zero-field splitting of the ground state into the magnetic sublevels. The combination of the large magnetic anisotropy with strong spin-orbital interactions leads to the SIMs behaviours.

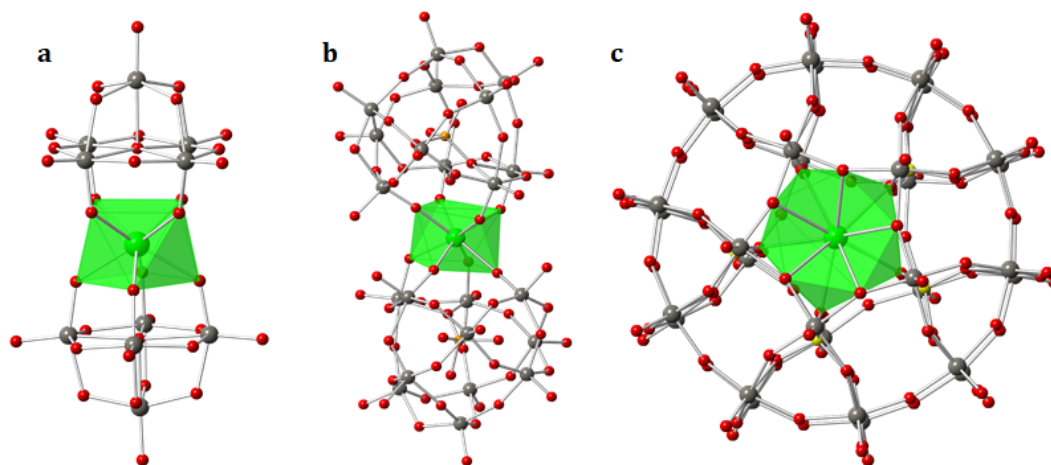
The first examples of Ln-based SIMs reported are from the LnPc₂ family, which was proposed in 2003 by Ishikawa and co-workers.¹ They successfully demonstrated that slow magnetic relaxation could occur in mononuclear lanthanide complexes, such as those in which a Ln ion is sandwiched between two Pc ligands, formulated as (Bu₄N)[LnPc₂] (Ln³⁺ = Tb³⁺ or Dy³⁺, Bu₄N = tetrabutylammonium) (Supplementary Fig. 2a). Later on, a massive synthetic effort has led to an ever-increasing number of compounds from the LnPc₂ family, which includes the introduction of a wide range of substituents at the periphery of the Pc macrocycles without significantly interfering with the metal binding properties of the ligands.^{20–24} Some structure representations of examples from this family studied in this work are shown below (Supplementary Fig. 2), as the sandwich complex [Bu₄N][DyPc(OTBPP)], (Supplementary Fig. 2b) in which one of the nitrogen atoms of one porphyrin pyrrole is replaced by an oxygen atom. Compared with the typical LnPc₂ complex, the atom replacement significantly enhances the effective energy barrier of the SIMs.²⁴ Another example is the use of tetraazaporphyrins (or porphyrazines) in place of the bulkier Pc ligands, giving rise to a series of neutral double-decker complexes that show analogous magnetic features as their Pc counterparts (Supplementary Fig. 2c).²⁵



Supplementary Figure 2 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of some cases from the LnPc_2 family. **a**, $[\text{Pc}_2\text{Ln}]^-$ from reference [1]. **b**, The sandwich-type mixed phthalocyaninato with core-modified porphyrinato double-decker complexes $[\text{DyPc}(\text{OTBPP})]^+$ or $[\text{Dy}(\text{Pc})(\text{STBPP})]^+$ from reference [24]. **c**, $[\text{Ln}(\text{OETAP})_2]^+$, where OETAP is octa(ethyl)tetraazaporphyrin.²⁵ (Color code: grey sphere, C; green sphere and polyhedron, Ln; blue sphere, N.)

2.2. POM family

The second representative family consists of polyoxometalates (POMs). This family contains all compounds where Ln^{3+} ions coordinate with POM ligands, including the cases where the coordination sphere is completed with other ligands. POMs are molecular metal-oxo clusters with early transition metals (W, Mo, Nb, Ta or V) in their highest oxidation states. The ability of these inorganic species to incorporate almost any kind of metal or non-metal addenda heteroatoms, together with their enormous molecular and electronic structural diversity, makes them of relevance in the molecular magnetism field. One relevant feature of POM ligands is that their diamagnetic structures can encapsulate Ln ions with coordination geometries similar to those of bis(phthalocyaninato)lanthanide complexes from LnPc_2 family.¹ More recently, POMs were used as extremely versatile inorganic building blocks for the construction of SMMs based either on $3d$ or $4f$ metal ions.²⁶ Some representative cases of complexes included in this study are shown below in Supplementary Fig. 3. The first example from the POM family exhibiting SIM behaviour is $[\text{ErW}_{10}\text{O}_{36}]^{9-}$ (Supplementary Fig. 3a).² Later on, two families of POM-based SIMs with formula $[\text{Ln}(\text{W}_5\text{O}_{18})_2]^{9-}$ and $[\text{Ln}(\beta_2\text{-SiW}_{11}\text{O}_{39})_2]^{13-}$ (Supplementary Fig. 3b) are reported in 2009, both of which show slow relaxation of the magnetisation, typical of the SIM-like behaviour.³ Another well-known series of complexes is $[\text{LnP}_5\text{W}_{30}\text{O}_{110}]^{12-}$ (Supplementary Fig. 3c), in which its unusual C_5 axial symmetry allows the study of new SIMs having 5-fold symmetry. The Dy^{3+} and Ho^{3+} derivatives exhibit SIM behaviour.⁴



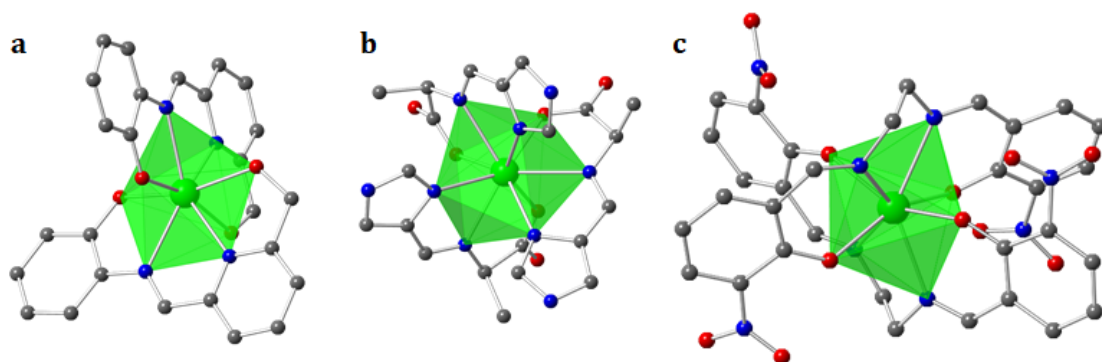
Supplementary Figure 3 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of three representative cases from the POM family. a, $[\text{ErW}_{10}\text{O}_{36}]^{9-}$ from reference [2]. **b,** $[\text{Ln}(\beta_2\text{-SiW}_{11}\text{O}_{39})_2]^{13-}$ from reference [3]. **c,** $[\text{LnP}_5\text{W}_{30}\text{O}_{110}]^{12-}$ from reference [4]. (Color code: grey sphere, W; green sphere and polyhedron, Ln; red sphere, O; yellow sphere, P; orange sphere, Si.)

2.3. Schiff base family

The third family is based on Schiff base ligands. This includes all samples where the Ln^{3+} ion coordinates to only Schiff base ligands; in addition, we included the cases where the strategy pursued by the authors (as stated in the title) relies on Schiff base ligand, even if other small ligands are used to complete the coordination sphere. Schiff base ligands are polydentate macrocyclic or macro-acyclic ligands, which typically contain both nitrogen and oxygen donors. However, the donor atom can be varied between sulfur, phosphorus, nitrogen, and oxygen. Due to their facile synthesis, Schiff base ligands are considered to be “privileged ligands”, which can easily make a coordination bond with many different metal ions and stabilize them in various oxidation states. In addition, when two equivalents of salicylaldehyde are combined with a diamine, a particular chelating Schiff base is produced, which is called salen ligands. Salen ligands present four coordinating sites (tetradentate) and two axial sites that are open to ancillary ligands, thus similar to porphyrins but with an easier preparation process.

Schiff bases derived from condensation reactions of aromatic aldehydes with primary amines have been the subject of extensive research because of their enormous versatility with respect to the formation of metal complexes with sophisticated discrete or expanded architectures and functional properties. The choice of initial reagents for the condensation determines the ligand coordination fashion and allows one to utilize both chelate and bridging functions of the obtained Schiff base. Schiff base complexes continue to intrigue chemists regarding their structure and reactivity. Their geometries are strongly influenced by the ligands and tend to be five- or six-coordinate. The first case listed here comprises two mono-deprotonated Schiff base $[\text{LH}]^-$ ligands, showing SIM behaviour and with a U_{eff} of 44.4 K in presence of a dc field

(Supplementary Fig. 4a).²⁷ Another case from this family is the Dy³⁺ complex with tridentate NNO ligands of N-[(imidazol-4-yl)methylidene]-DL-alanine (Supplementary Fig. 4b), which shows an out-of-phase signal with frequency-dependence in ac susceptibility under a dc bias field of 10³ Oe, indicative of field induced SIM.²⁸ One other representative case from this family is the Salen-type mononuclear Ln³⁺ complex [Ln(3-NO₂-salen)₂]⁻ (Supplementary Fig. 4c), which shows slow magnetisation relaxation processes associated with SIM behaviour.²⁹

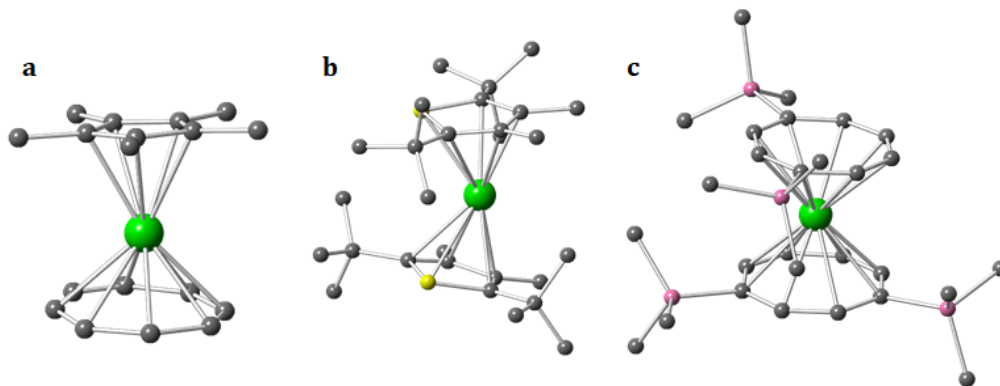


Supplementary Figure 4 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of some cases from the Schiff base family. a, [Ln(LH)₂]⁻ where H₂L = 2-(((6-(hydroxymethyl)pyridin-2-yl)-methyleneamino)phenol).²⁷ b, ‘fac’-[Dy^{III}(HL^{DL-ala})₃], where H₂L^{DL-ala} is N-[(imidazol-4-yl)methylidene]-DL-alanine.²⁸ c, [Ln(3-NO₂-salen)₂]⁻, where Ln can be Dy, Er or Yb, and 3-NO₂-salen²⁻ = N,N'-bis(3-nitro-salicylaldehyde)ethylenediamine dianion.²⁹ (Color code: grey sphere, C; green sphere and polyhedron, Ln; red sphere, O; blue sphere, N.)

2.4. Metallocene family

The fourth family is based on the small aromatic ligands derived from conjugated hydrocarbon ligands, typically cyclopentadienyl or cyclooctatetraene anions. We only include in this classification the complexes where the coordination sphere is completed by this kind of ligands, in contrast with cases with an extra “equatorial” coordination site. Compared with heteroatomic donor atoms such as oxygen and nitrogen, which have limited orbital overlap with the shielded 4*f* orbitals, the aromatic ligands allow the perturbation of the crystal field of the lanthanide ions through the use of an electron π -cloud. Thus, it can further control over the anisotropic axis and induction of *f-f* interactions, making donor atoms as conjugated hydrocarbons.³⁰ Here we list some examples by employing delocalized ligands to design SIMs with prominent uniaxial anisotropy. An Er³⁺ ion sandwiched by two aromatic ligands, pentamethylcyclopentadienide anion (C₅Me₅⁻, Cp*) and cyclooctatetraenide dianion (C₈H₈²⁻, COT) (Supplementary Fig. 5a), displays a butterfly-shaped hysteresis loop at 1.8 K up to even 5 K.³¹ Another example is a bis-monophospholyl Dy³⁺ SIM, [Dy(Dtp)₂][Al{OC(CF₃)₃}₄] (Supplementary Fig. 5b), which shows an effective energy barrier to magnetisation reversal of 1760 K (1223 cm⁻¹) and magnetic

hysteresis up to 48 K.³² The use of planar cyclooctatetraenide (COT^{2-}) ligands allows the access to the sandwich type complex $[\text{Dy}(\text{COT}'')_2]\text{Li}(\text{DME})_3$ (Supplementary Fig. 5c), which exhibits slow relaxation of the magnetisation indicating its SIM behaviour.³³

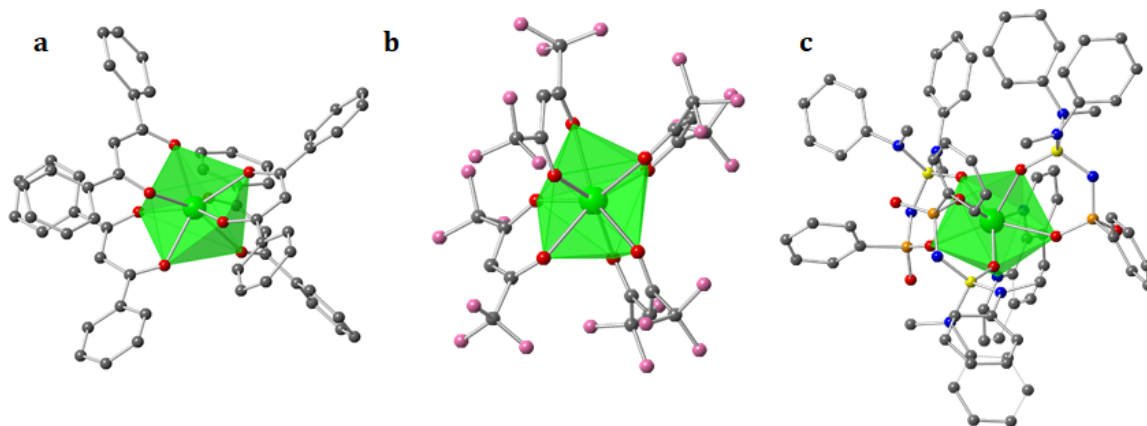


Supplementary Figure 5 | Ball-and-stick models of the coordination spheres around Ln^{3+} ions of some cases from the metallocene family. **a**, $(\text{Cp}^*)\text{Er}(\text{COT})$, where $\text{Cp}^* = \text{C}_5\text{Me}_5^-$ and $\text{COT} = \text{C}_8\text{H}_8^{2-}$, from reference [31]. **b**, $[\text{Dy}(\text{Dtp})_2][\text{Al}\{\text{OC}(\text{CF}_3)_3\}_4]$, where $\text{Dtp} = \{\text{P}(\text{C}'\text{BuCMe})_2\}$.³² **c**, $[\text{DyCOT}''_2]$, where $\text{COT}'' = \text{cyclooctatetraenide rings}$.³³ (Color code: grey sphere, C; green sphere, Ln; pink sphere, Si; yellow sphere, P.)

2.5. Diketonate family

The fifth family is the diketonate family of complexes, it includes those samples with Ln^{3+} ions coordinated with diketonate ligands and diketonate ligands mixed with other molecules which are not defined in the classification. The diketonate ligands are bidentate and bond through delocalized chelate rings formed through two oxygen atoms. β -diketone SIMs have received much attention in recent years, since β -diketone can provide a stable bidentate chelating mode to afford eight-coordinated mononuclear lanthanide complexes. There are two different polyhedron coordination geometries for the β -diketone complexes, square antiprism with D_{4d} symmetry and triangular dodecahedron with D_{2d} symmetry. After the SMM behaviour of a simple acetylacetonate complex has been reported on several β -diketone complexes, much effort is devoted to the synthesis and investigation of β -diketone SIMs. In addition to the coordination geometry, the stability of the SIMs upon heating is also an important topic. Lanthanide β -diketone complexes with fluorides as substituent groups, such as hexafluoroacetylacetonate (hfac), can make the complexes stable upon heating. By using the β -diketonate ligand dibenzoylmethane (DBM) anion, mononuclear Dy complex $[\text{Hex}_4\text{N}][\text{Dy}(\text{DBM})_4]$ (Supplementary Fig. 6a) was obtained, in which slow magnetic relaxation is observed.¹⁶ A typical compound of β -diketone is formulated as (cation) $[\text{Ln}(\beta\text{-diketone})_4]$, in which the Ln^{3+} ion is surrounded by four β -diketone forming a LnO_8 environment. The complex shown in Supplementary Fig. 6b, using hfac ligand, exhibits field-induced slow magnetization relaxation.¹⁷ Another case is the use of a sulfonyl amidophosphate (SAPh), acting as a β -diketone homologue

for the complexation of Ln ion, which gives rise to complex LnL_3Phen ($\text{L} = \text{C}_6\text{H}_5\text{SO}_2\text{NP}(\text{O})[\text{N}(\text{CH}_3)(\text{C}_6\text{H}_5)]_2$) with in-field SIM behaviours (Supplementary Fig. 6c).³⁴

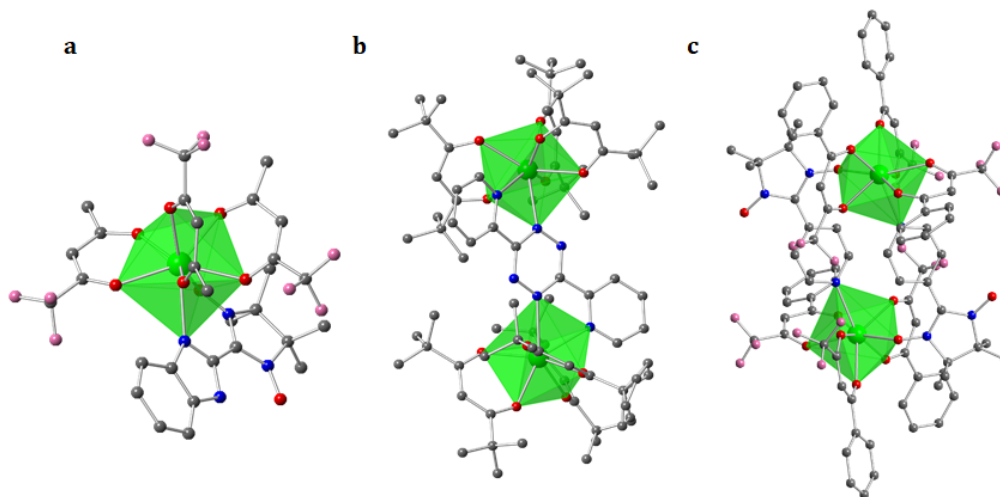


Supplementary Figure 6 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of some cases from the diketonate family. **a**, $[\text{Dy}(\text{DBM})_4]^-$, where DBM = dibenzoylmethane anion ligand.¹⁶ **b**, $\{\text{Dy}(\text{hfac})_4\}$, where hfac = hexafluoroacetylacetone.¹⁷ **c**, $[\text{LnL}_3(\text{phen})]$, where Ln can be Dy or Er, and L is deprotonated bis(methyl(phenyl)amino)phosphoryl)-benzenesulfonamide, $\text{C}_6\text{H}_5\text{SO}_2\text{NP}(\text{O})[\text{N}(\text{CH}_3)(\text{C}_6\text{H}_5)]_2$, and Phen = phenanthroline.³⁴ (Color code: grey sphere, C; green sphere and polyhedron, Ln; red sphere, O; yellow sphere, P; pink sphere, F; blue sphere, N; orange sphere, S.)

2.6. Radical family

The sixth family is composed of complexes in which Ln^{3+} ion is coordinated with radical-based ligand(s), such as nitronyl nitroxide and semiquinones. Radical ligands are one of the most efficient bridging ligands for the design of molecular magnetic materials.³⁵ The radical systems are relatively abundant in our dataset, being more numerous than any other family presented so far. The reason of choosing radical ligands is that they possess $2p$ diffuse spin orbitals that can potentially penetrate the core electron density of the lanthanide ions to reach deeply buried $4f$ orbitals, whose shielded magnetic orbitals are usually a drawback for their use in extended magnetically coupled structures.³⁶ The strong $2p$ - $4f$ heterospin exchange coupling effectively shifts degenerated m_J sublevels to different energies and, furthermore, significantly reduces the probability of resonant quantum tunnelling and lengthens the relaxation time. We will show some examples from this family (Supplementary Fig. 7). The first case is the nitronyl nitroxide radical complex $[\text{Ln}(\text{tfa})_3(\text{NIT-BzImH})]$, (Supplementary Fig. 7a) in which Ln^{3+} ion is 8-coordinated to one NIT-BzImH and three trifluoroacetylacetone (tfa) ligands. It shows slow magnetic relaxation suggesting that they behave as SIMs.¹⁰ The second case is a dinuclear Ln^{3+} compound with its formula as $\{\text{Cp}_2\text{Co}\}\{\text{[Dy}(\text{tmhd})_3]_2(\text{bptz})\}$ in radical anion form (Supplementary Fig. 7b), in which the rare earth ions are isolated by an organic ligand bridged species. It exhibits out-of-phase ac susceptibility signals below 4 K.¹⁵ Another relevant case is a

cyclic dimer structure, in which each pyridine substituted radical links two different metal ions through the oxygen of a nitroxide group and the pyridine nitrogen (Supplementary Fig. 7c). It shows frequency-dependent ac magnetic susceptibility, indicating SIM behaviour.⁹

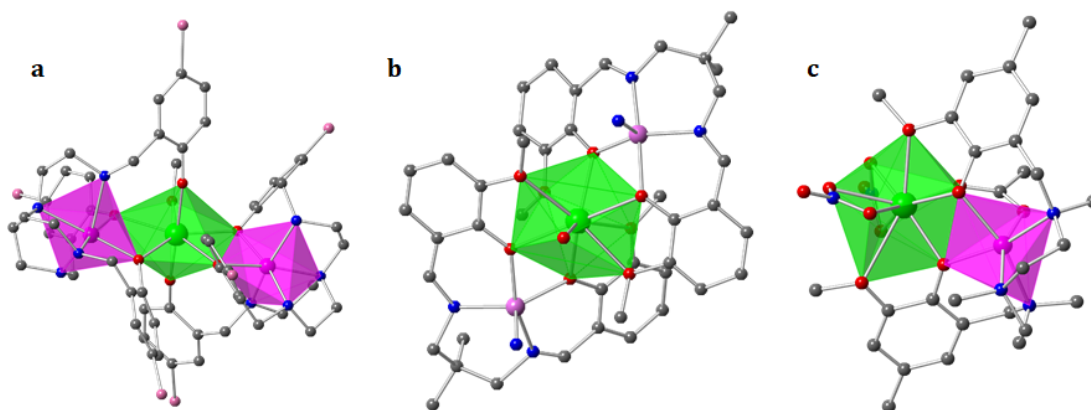


Supplementary Figure 7 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of some cases from the radical family. **a**, $[\text{Ln}(\text{tfa})_3(\text{NIT-BzImH})]$, where tfa = trifluoroacetylacetonate; NIT-BzImH = 2-(2'-benzimidazolyl)-4,4,5,5-tetramethylimidazolyl-1-oxyl-3-oxide.¹⁰ **b**, $\{\text{Cp}_2\text{Co}\} \{[\text{Dy}(\text{tmhd})_3]_2(\text{bptz})\}$, where tmhd = 2,2,6,6-tetramethyl-3,5-heptane dionate and bptz = 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine.¹⁵ **c**, $[\text{Ln}(\text{Phtfac})_3(\text{NITpPy})]_2$, where HPhtfac = 4,4,4-trifluoro-1-phenylbutane-1,3-dione and NITpPy = 2-(4-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxyl-3-oxide.⁹ (Color code: grey sphere, C; green sphere and polyhedron, Ln; red sphere, O; pink sphere, F; blue sphere, N.)

2.7. TM near Ln family

This family of complexes is defined when a diamagnetic transition metal (TM) ion exists in the coordination sphere of Ln^{3+} ion. There are several Ln-based SIMs containing one or more 3d metal ions.^{37–40} Most of this type of complexes contain Schiff base ligand or a diketone ligand.³⁷ For example, Yamashita *et al.* reported an Er-based SIM,⁴¹ where the Er^{3+} ion is coordinated with a Schiff base ligand, which in turn is connected to the diamagnetic transition metal Zn^{2+} through oxygen. Macrocyclic ligands provide discrete metal binding pockets and, therefore, offer a more predictable cluster nuclearity and structure than acyclic analogues can.³⁷ For example, the [3+3] macrocycle provides three N_2O_2 pockets for 3d metal ions and one central O_6 pocket for a Ln ion, making mixed-metal M_3Ln tetrametallic macrocyclic complexes predictable.^{41,42} Macrocycles usually provide enhanced stability, solubility and fine-tunability (vary the choice of M and Ln, whilst retaining the M_3Ln core) over acyclic analogues. It's documented that the U_{eff} of Ln-based SIMs can be enhanced by introducing diamagnetic metal ions in the coordination sphere. The

diamagnetic ion may induce large electrostatic interaction between the Ln^{3+} ion and coordination atoms, giving rise to the destabilization of excited states and increasing the gap between the ground state and the first excited state.^{43–45} There are many compounds that fall into the “diamagnetic TM near the Ln center” category. For instance, the pentagonal-bipyramid (quasi- D_{5h}) $[\text{Zn}–\text{Dy}–\text{Zn}]$ complex (Supplementary Fig. 8a) exhibits a large thermally activated barrier with long relaxation times.⁴⁵ Other cases are $\{[\text{Zn}(\text{Me}_2\text{valpn})]_2\text{Dy}(\text{H}_2\text{O})\text{Cr}(\text{CN})_6\}_2$ (Supplementary Fig. 8b)⁴⁰ and $[\text{Zn}(\mu\text{-L})(\mu\text{-OAc})\text{Er}(\text{NO}_3)_2]$ (Supplementary Fig. 8c)⁴⁶, both exhibit SIM behaviour.

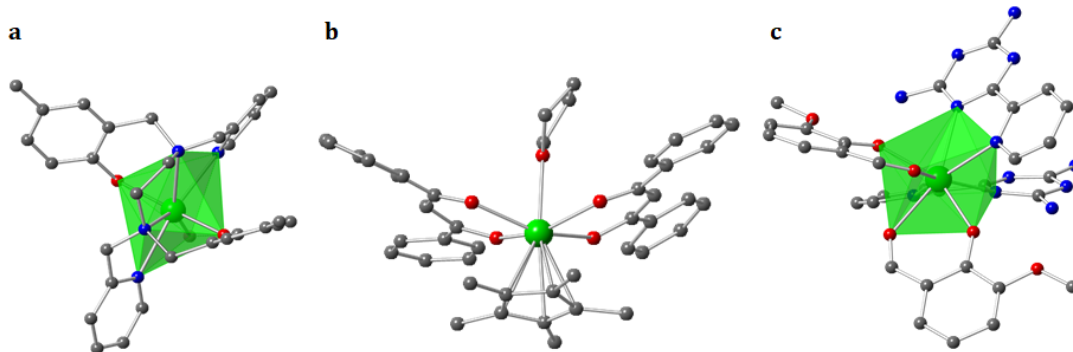


Supplementary Figure 8 | Combined polyhedral and ball-and-stick representations of the coordination spheres around Ln ions of examples from the TM near Ln family. **a**, $[\text{Zn}_2\text{DyL}_2(\text{MeOH})]^-$, where L is 2,2',2''-(((nitrilotris(ethane-2,1-diyl))tris(azanediyl))tris(methylene))tris-(4-bromophenol).⁴⁵ **b**, $\{[\text{Zn}(\text{Me}_2\text{valpn})]_2\text{Dy}(\text{H}_2\text{O})\text{Cr}(\text{CN})_6\}_2$, where $\text{Me}_2\text{valpn}^{2-}$ is dianion of N,N'-2,2-dimethylpropylenebis(3-methoxysalicylideneimine).⁴⁰ **c**, $[\text{Zn}(\mu\text{-L})(\mu\text{-OAc})\text{Er}(\text{NO}_3)_2]$, where H_2L is N,N',N''-trimethyl-N,N''-bis(2-hydroxy-3-methoxy-5-methylbenzyl)diethylenetriamine.⁴⁶ (Color code: grey sphere, C; green sphere and polyhedron, Ln; magenta sphere and polyhedron, Zn; red sphere: O; pink sphere, Br; blue sphere: N.)

2.8. Mixed ligands family

The eighth category is defined as mixed ligands. It contains all cases where the Ln^{3+} ion is coordinated with one kind of ligands defined above together with another ligand not defined, thus, mixed ligands. The design strategy of using mixed ligands for high performance SIMs is promising. There are many complexes from this category which possess SIM behaviour. One example is using N,N'-bis(2-hydroxybenzyl)-N,N'-bis(2-methylpyridyl)ethylenediamine and Cl (or Br) as ligands for synthesis of the seven-coordinate complex $[\text{Dy}(\text{bbpen-CH}_3)\text{X}]$, which produces high performance SIMs (Supplementary Fig. 9a).⁴⁷ Another representative case is the half-sandwich organometallic complex $[\text{Cp}^*\text{Dy}(\text{DBM})_2(\text{THF})]$ (Supplementary Fig. 9b) with a

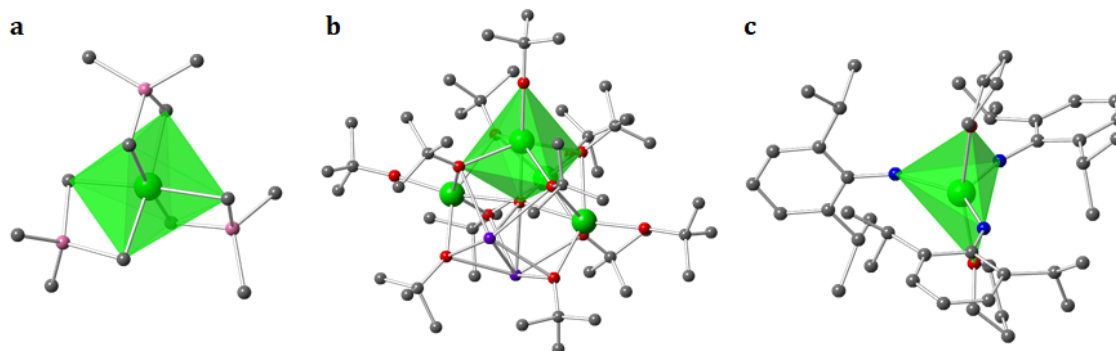
Janus structural motif, where the ligands are composed of THF, DBM⁻ and [Cp*]⁻. It displays slow magnetic relaxation in the absence of an applied magnetic field, indicating SIMs properties.⁴⁸ By combination of β -diketonate with 6-pyridin-2-yl-[1,3,5]triazine-2,4-diamine ligands, a series of SIMs were obtained and investigated (Supplementary Fig. 9c).⁴⁹



Supplementary Figure 9 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of some cases from the mixed ligands family. **a**, [Dy(bbpen-CH₃)X], where X = Cl or Br and H₂bbpen = N,N'-bis(2-hydroxybenzyl)-N,N'-bis(2-methylpyridyl)ethylenediamine.⁴⁷ **b**, [Cp*Dy(DBM)₂(THF)], where Cp* = C₅Me₅⁻ and DBM = dibenzoylmethanoate anion.⁴⁸ **c**, [DyLz₂(o-vanilin)₂]⁺, where Lz = 6-pyridin-2-yl-[1,3,5]triazine-2,4-diamine and X = Br⁻, NO₃⁻, CF₃SO₃⁻, from reference [49]. (Color code: grey sphere, C; green sphere and polyhedron, Ln; red sphere, O; blue sphere, N.)

2.9. Other families

The last category is named as “other families”. It includes all complexes which fall into the criterion of complex selection but the coordination ligands of Ln ions are not in the ligand families previously defined. Large numbers of complexes included in this work are from this category. For instance, the octahedral dysprosium aluminate complex [Dy(AlMe₄)₃] shows fast relaxation of the magnetisation via quantum tunnelling (Supplementary Fig. 10a).⁵⁰ Also, the alkoxide cage complexes [DyY₃K₂O(O^{*i*}Bu)₁₂] and [DyY₄O(O^{*i*}Pr)₁₃] (Supplementary Fig. 10b) incorporate a small amount of DyCl₃ in the synthesis of [Dy₄K₂O(O^{*i*}Bu)₁₂] and [Dy₅O(O^{*i*}Pr)₁₃] to produce {DyY₃K₂} in a {Y₄K₂} matrix, or {DyY₄} in {Y₅}. These complexes show a single dominant relaxation process with very high U_{eff} values.⁵¹ Another relevant cases are the five-coordinate complexes Ln(NHPh^{*i*}Pr)₃(THF)₂, (Ln = Dy and Er), with trigonal bipyramidal geometry, both of which exhibit slow magnetic relaxation under a zero/non-zero dc applied magnetic field (Supplementary Fig. 10c).⁵²



Supplementary Figure 10 | Combined polyhedral and ball-and-stick models of the coordination spheres around Ln ions of three examples from the other families. a, $[\text{Dy}(\text{AlMe}_4)_3]$ from reference [50]. **b,** $[\text{DyY}_3\text{K}_2\text{O}(\text{O}'\text{Bu})_{12}]$ from reference [51]. **c,** $\text{Ln}(\text{NHP}'\text{Pr}_2)_3(\text{THF})_2$, in which Ln^{3+} can be Dy^{3+} or Er^{3+} , from reference [52]. (Color code: grey sphere, C; green sphere and polyhedron, Ln or Y^{3+} ; red sphere, O; blue sphere, N; pink sphere, Al.)

Supplementary Section 3. A graphical, interactive, browsable App

To facilitate a broader use by the chemical community of the data collected in the present study, we developed the tool SIMDAVIS (Single Ion Magnet DATA VISualization): a graphical, interactive, browsable online database of over 1400 samples. Employing SIMDAVIS, any user can study the data in different and complementary ways. The four modes of operation, accessible in different tabs within the program, are “ScatterPlots”, “BoxPlots”, “BarCharts” and “Data” table. There is also an information subtab denoted as “Variables” within the “About SIMDAVIS” tab in which the definition of each variable can be found.

The basic use of the “ScatterPlots” tab is the representation of quantitative data against each other, *e.g.* the maximum hysteresis temperature (T_{hyst}) vs the effective energy barrier (U_{eff}). This allows a visual estimate on the relation between different experimental and theoretical descriptors of the magnetic behaviour. Other relevant numerical variables in the dataset include T_{B3} , T_{B3H} , the alternate estimate for the effective energy barrier ($U_{\text{eff,ff}}$), or the pre-exponential factors τ_0 , $\tau_{0,\text{ff}}$, for either the simplistic equation or the full fit (see details about the variables in Supplementary Section 1). Furthermore, the “ScatterPlots” tab allows to distinguish the data points plotted according to a number of qualitative (categorical) variables, which can be of chemical nature, such as the chemical family, or which lanthanide ion was employed. Also, you may distinguish the points by some categorical variables of physical nature, such as presence or absence of magnetic memory above 2 K, in form of hysteresis or maximum in the χ'' (categorical variable χ''_{max} in our dataset). It also allows the user to select or deselect the represented data depending on these qualitative variables, to help distinguish quantitative correlations that might be different for different classes of compounds. Finally, there is also an option to fit linear

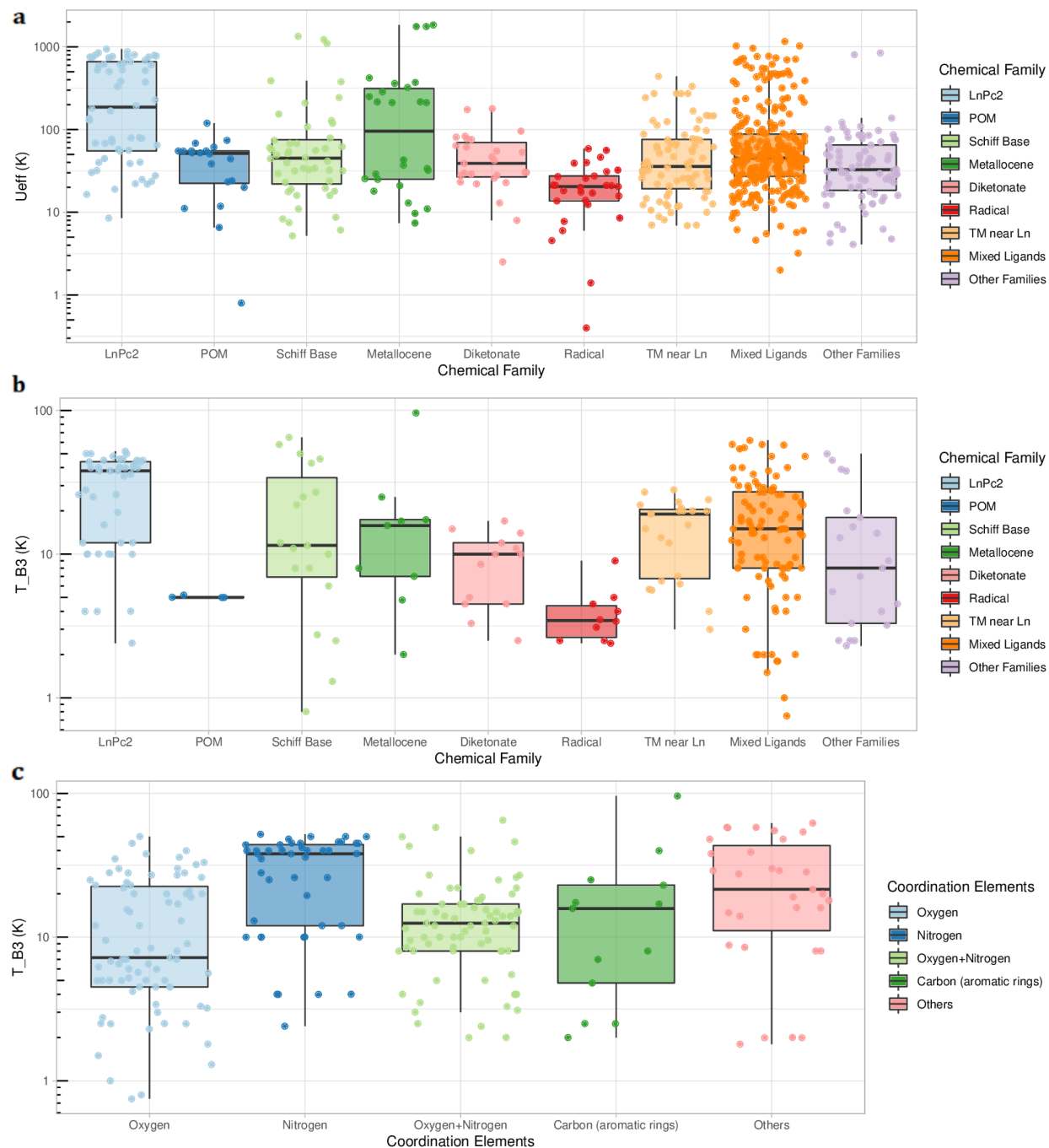
regressions between the two represented quantitative variables for each of the categorical classes. These variations can combine to hundreds of thousands of distinct meaningful plots.

The “BoxPlot” tab allows a different type of representation. One can plot the values of any of the quantitative variables *vs* any of the qualitative variables, for a total of 108 possible variable pairs producing distinct representations. The distribution of a single quantitative variable (*e.g.* U_{eff}) is represented, showing the data points, the median, the low (first or Q1) quartile, upper (third or Q3) quartile, and whiskers. The upper whisker extends from the hinge to the largest value no further than 1.5xIQR from the hinge (where IQR is the interquartile range, or distance between the first and third quartiles). The lower whisker extends from the hinge to the smallest value at most 1.5xIQR of the hinge. This representation is done in parallel for different values of a qualitative variable, *e.g.* “Coordination Elements”. An advantage of these boxplots *vs* the more sophisticated scatterplots is a larger amount of data to be represented at any given time. Note that there is virtually no paper that contains simultaneously all the kinds of information recorded in the dataset. For example, only a minority of the papers have historically performed a full fit considering Orbach, Raman, quantum tunneling and/or direct mechanism of relaxation. This means that the scatter plots, by being restricted to samples where two particular quantitative data kinds are well defined, effectively work with less data, so while they enable us to extract more nuanced dependencies, inevitably some information is lost.

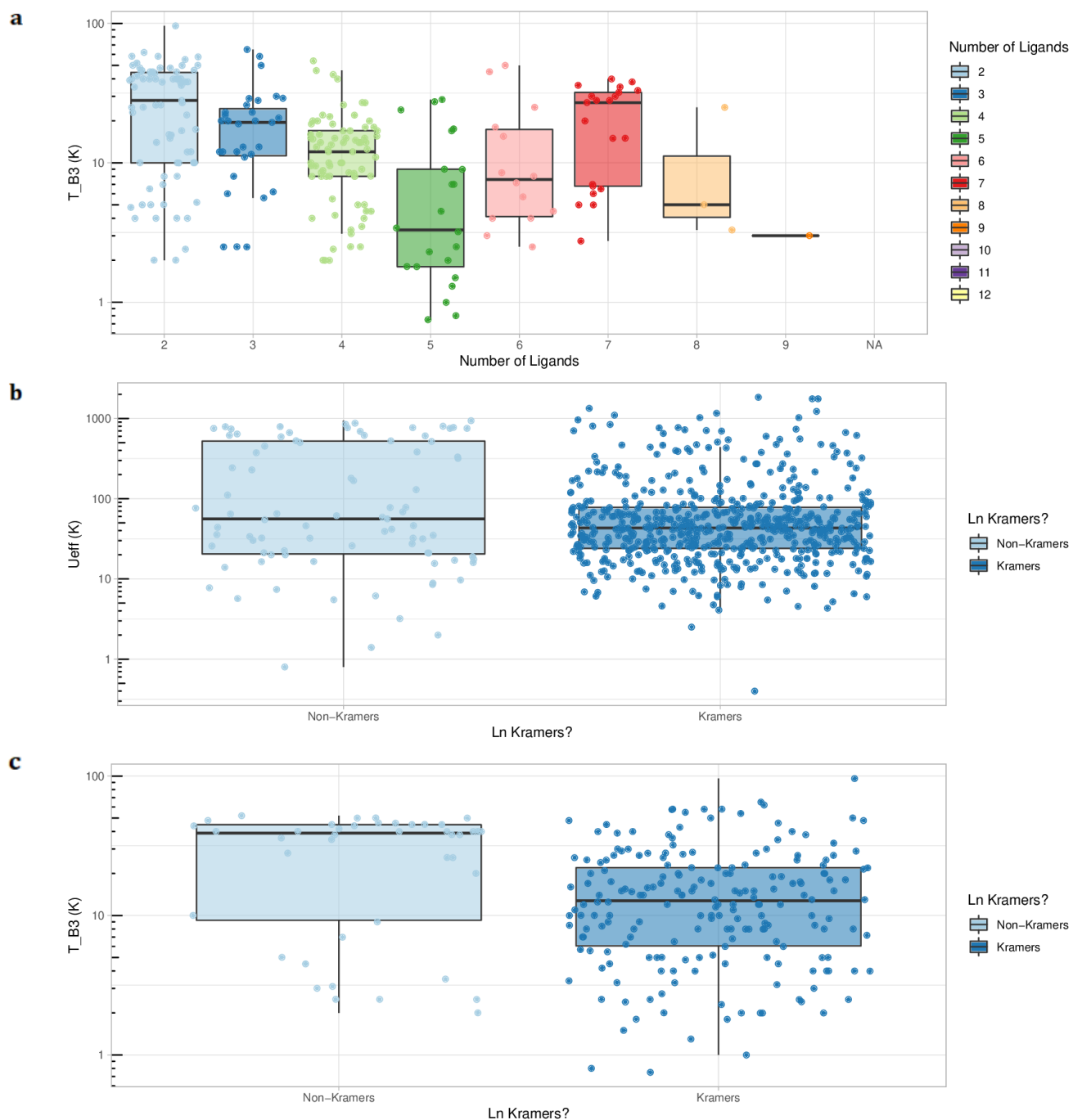
In the “BarCharts” tab, the different qualitative data types can be represented *vs* each other, for a total of 144 variable pairs producing distinct representations. Since qualitative information is available for almost all samples, bar charts contain almost all data points and allow for a quick frequency check of frequencies of different values in the dataset. Again, they provide a complementary mode of analysis of correlations. In our case, rather than the standard bar chart, SIMDAVIS employs stacked bar graphs meaning we can analyze the covariation of two variables, *e.g.* Tb^{3+} is more common in the SIM literature than Er^{3+} , but whereas this is especially true for the chemical families of “LnPc₂” and “radicals”, the reverse trend is found for the metallocene family.

The “Data” tab contains a mini-menu with two options: it allows the user to download the raw dataset, and it allows the user to browse the data set. The browsing is interactive in different, complementary ways. First, it allows the user to select the columns to show, *e.g.* by default each entry just shows 7 columns of data, namely the sample ID, formula of the compound, its chemical family, the Ln ion, the coordination elements, U_{eff} , and the DOI of the article where the information was obtained, while the other 24 columns are hidden. Second, it allows the user to arrange the information by ascending or descending order of the chosen variable. Finally, it includes a search tool that filters for text strings in real time.

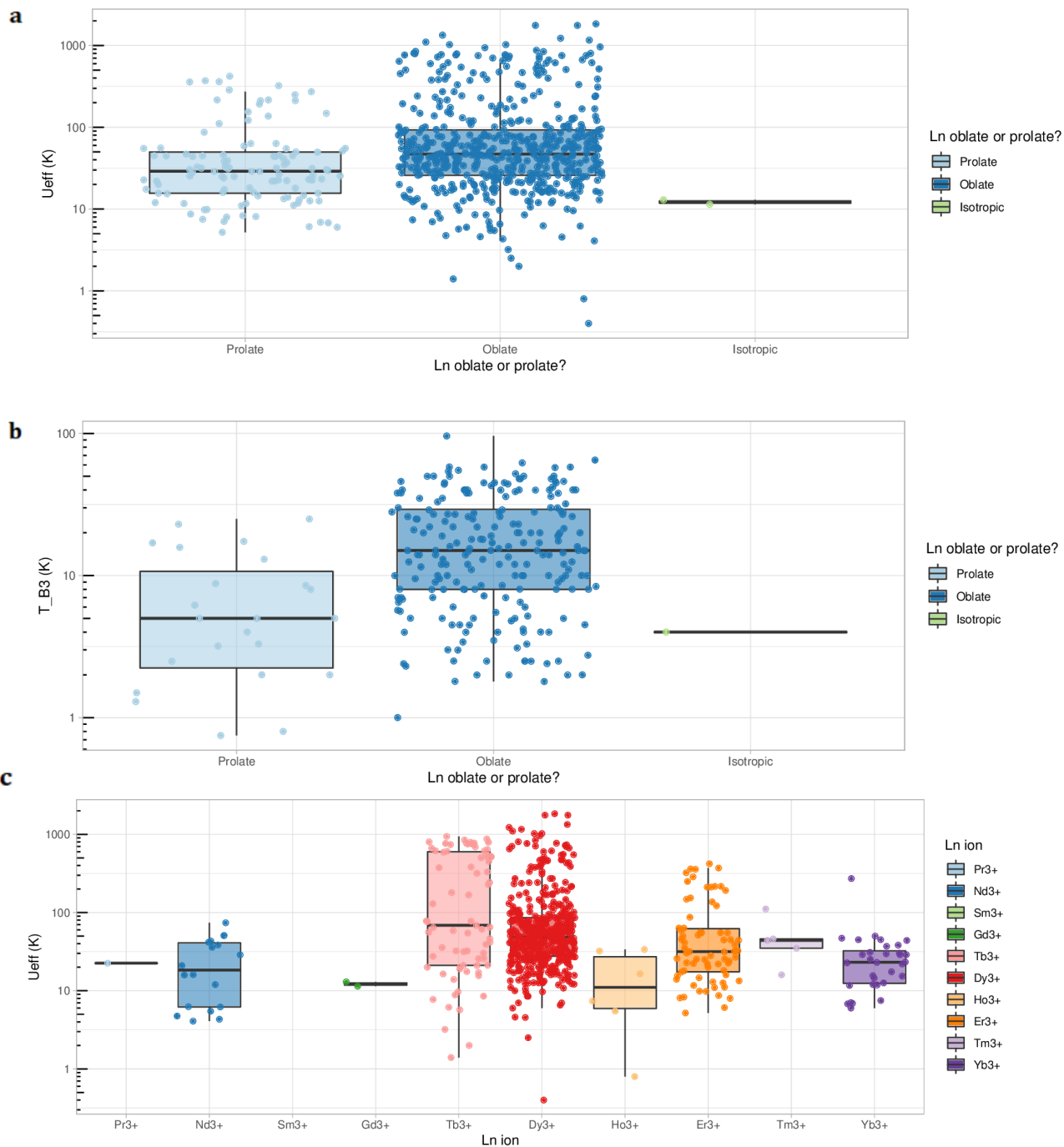
3.1. Gallery of SIMDAVIS graphs: chemical variables to optimize the physical properties



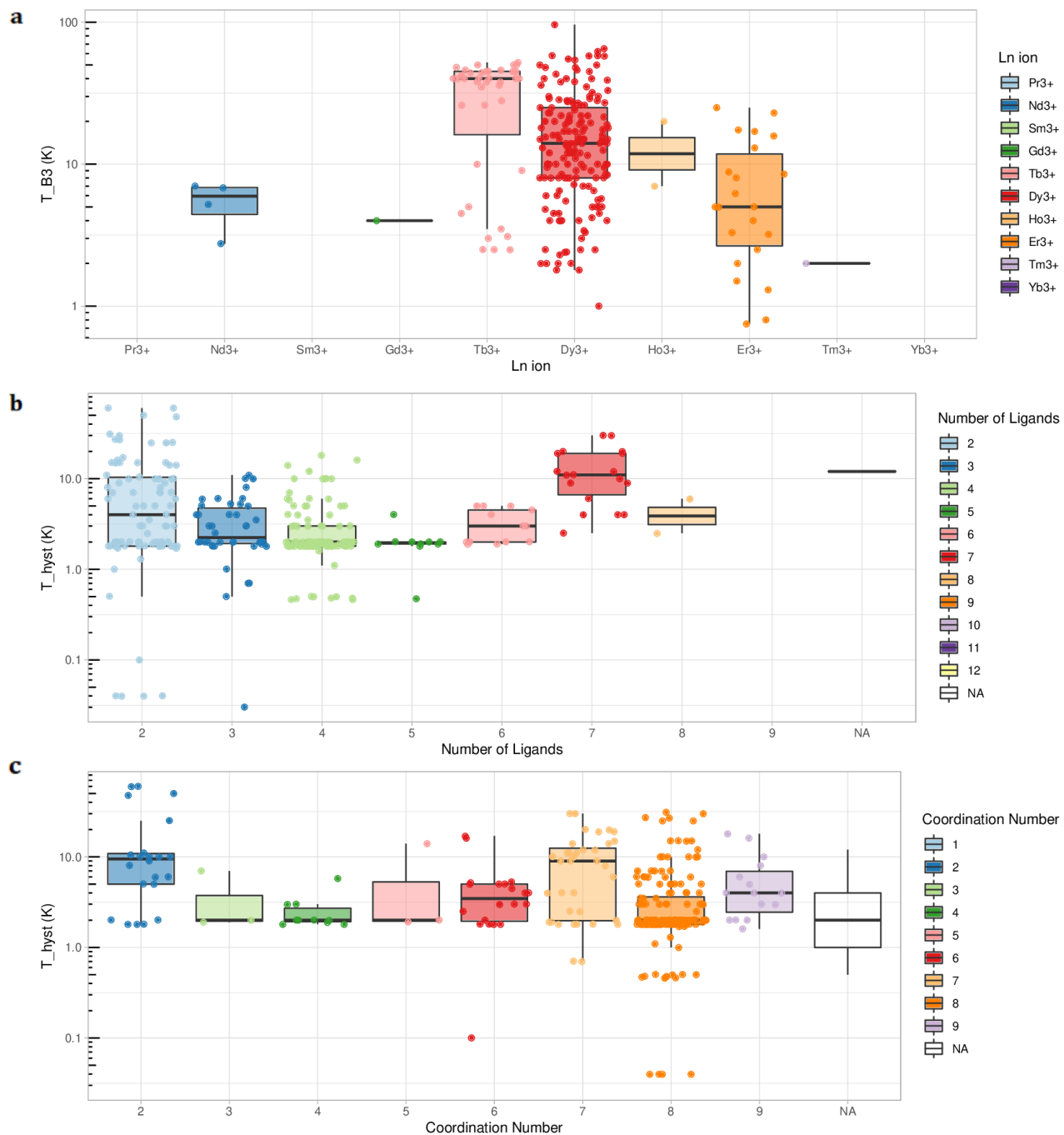
Supplementary Figure 11.1 | Boxplots of physical variables vs chemical variables. a, U_{eff} vs chemical family. b, T_{B3} vs chemical family. c, T_{B3} vs coordination elements.



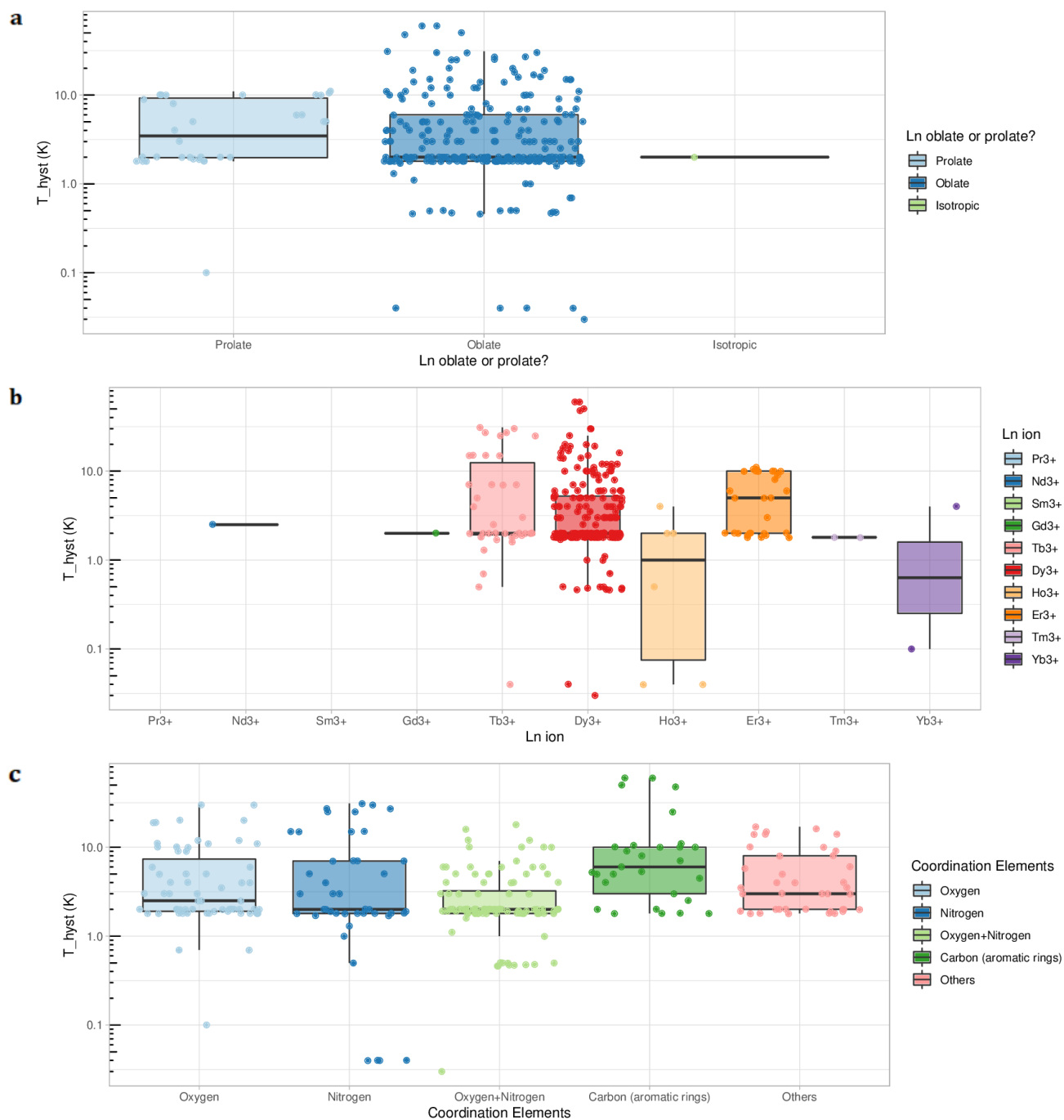
Supplementary Figure 11.2 | Boxplots of physical vs chemical variables. a, T_{B3} vs number of ligands. b, U_{eff} vs spin parity of the metal ion. c, T_{B3} vs spin parity of the lanthanide ion.



Supplementary Figure 11.3 | Boxplots of physical vs chemical variables. a, U_{eff} vs anisotropy of the lanthanide ion. b, T_{B3} vs anisotropy of the lanthanide ion. c, U_{eff} vs lanthanide ion.



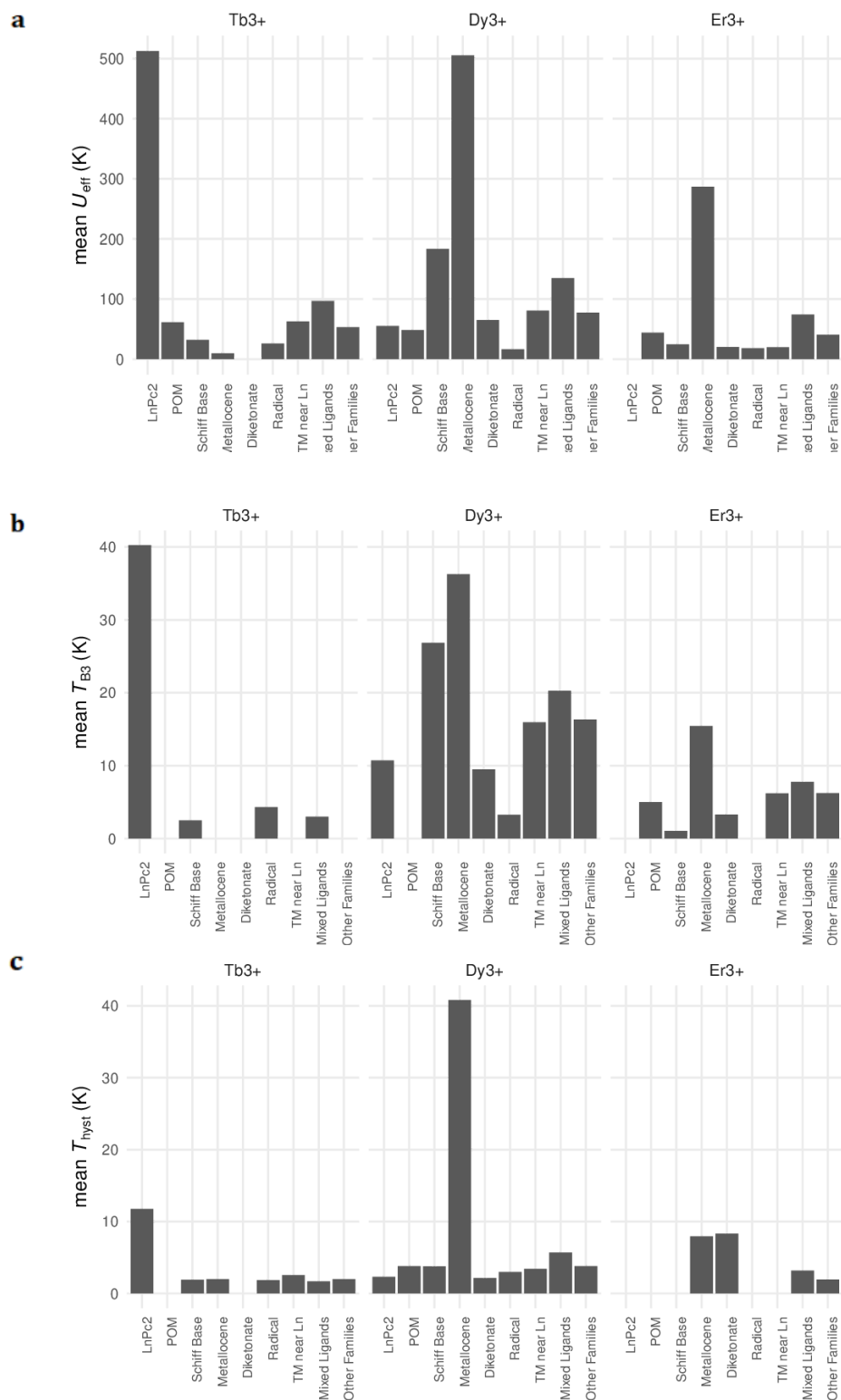
Supplementary Figure 11.4 | Boxplots of physical vs chemical variables. a, T_{B3} vs lanthanide ion. b, T_{hyst} vs number of ligands. c, T_{hyst} vs coordination number.



Supplementary Figure 11.5 | Boxplots of physical vs chemical variables. a, T_{hyst} vs anisotropy of the lanthanide ion. b, T_{hyst} vs lanthanide ion. c, T_{hyst} vs coordination elements.

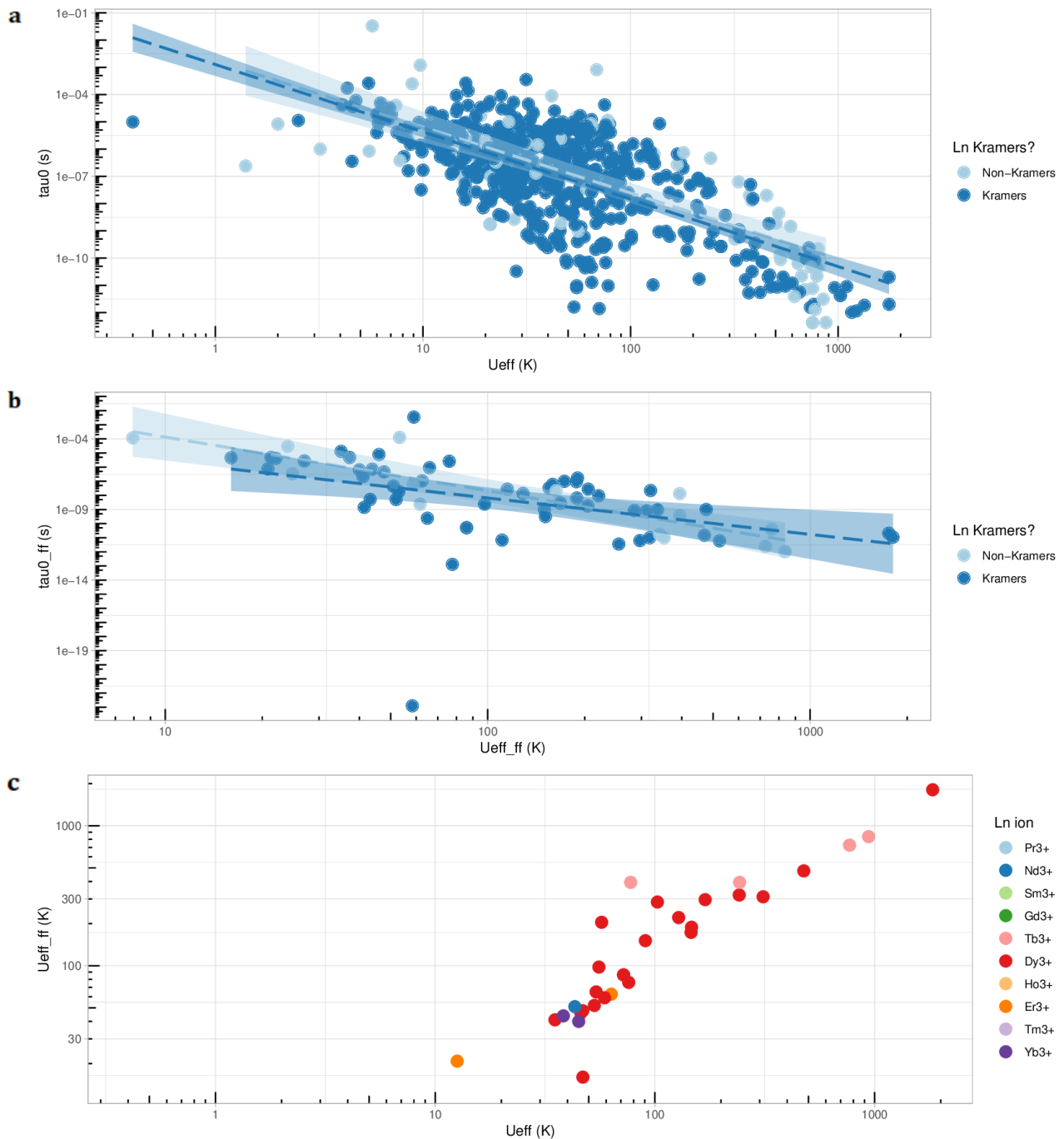


Supplementary Figure 11.6 | Boxplots of physical vs chemical variables. a, T_{hyst} vs chemical family. b, U_{eff} vs coordination elements.

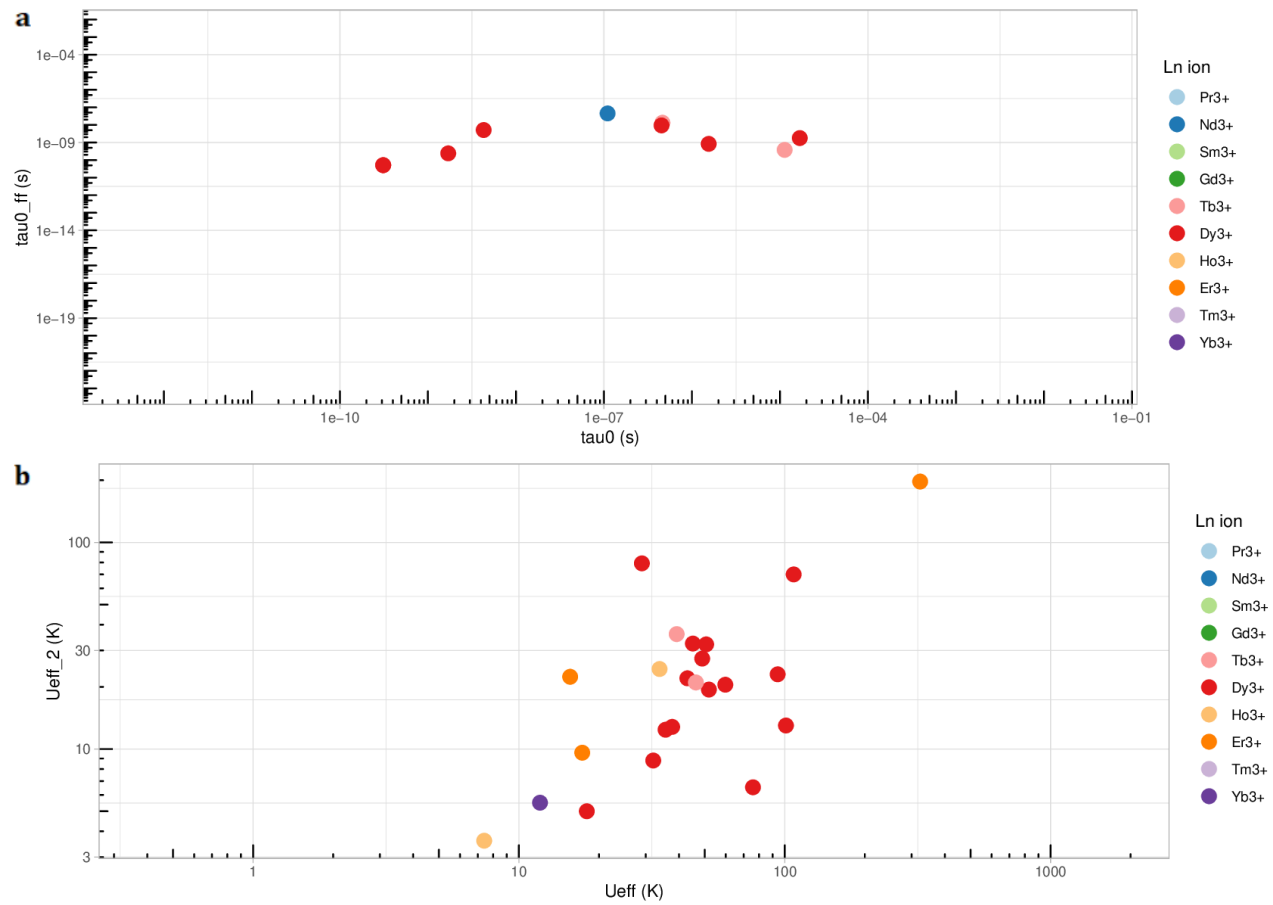


Supplementary Figure 12 | Bar chart representations of the relation between Ln ion, chemical family and arithmetic mean of U_{eff} , T_{B3} and T_{hyst} . Bar charts showing the mean values for every combination of categories between the main metal ions {Tb³⁺, Dy³⁺, Er³⁺} and all chemical categories. **a**, U_{eff} , **b**, T_{B3} , **c**, T_{hyst} .

3.2. Extended gallery of SIMDAVIS graphs: Arrhenius equation parameters



Supplementary Figure 13.1 Scatterplot representations of the relation between U_{eff} , $U_{\text{eff,ff}}$, τ_0 , $\tau_{0,\text{ff}}$. **a**, τ_0 vs U_{eff} , for Kramers and non-Kramers ions, with linear regressions; **b**, $\tau_{0,\text{ff}}$ vs $U_{\text{eff,ff}}$, for Kramers and non-Kramers ions, with linear regressions; **c**, $U_{\text{eff,ff}}$ vs U_{eff} for different lanthanide ions, with a visible linear behaviour.



Supplementary Figure 13.2 | Scatterplot representations of $\tau_{0,ff}$, $U_{eff,2}$ vs τ_0 , $U_{eff,ff}$. **a, $\tau_{0,ff}$ vs τ_0 for different lanthanide ions, with no discernible relation between the parameters; **b**, $U_{eff,2}$ vs U_{eff} for different lanthanide ions, with no discernible relation between the parameters.**

Supplementary Section 4. Statistical analysis of the chemical variables

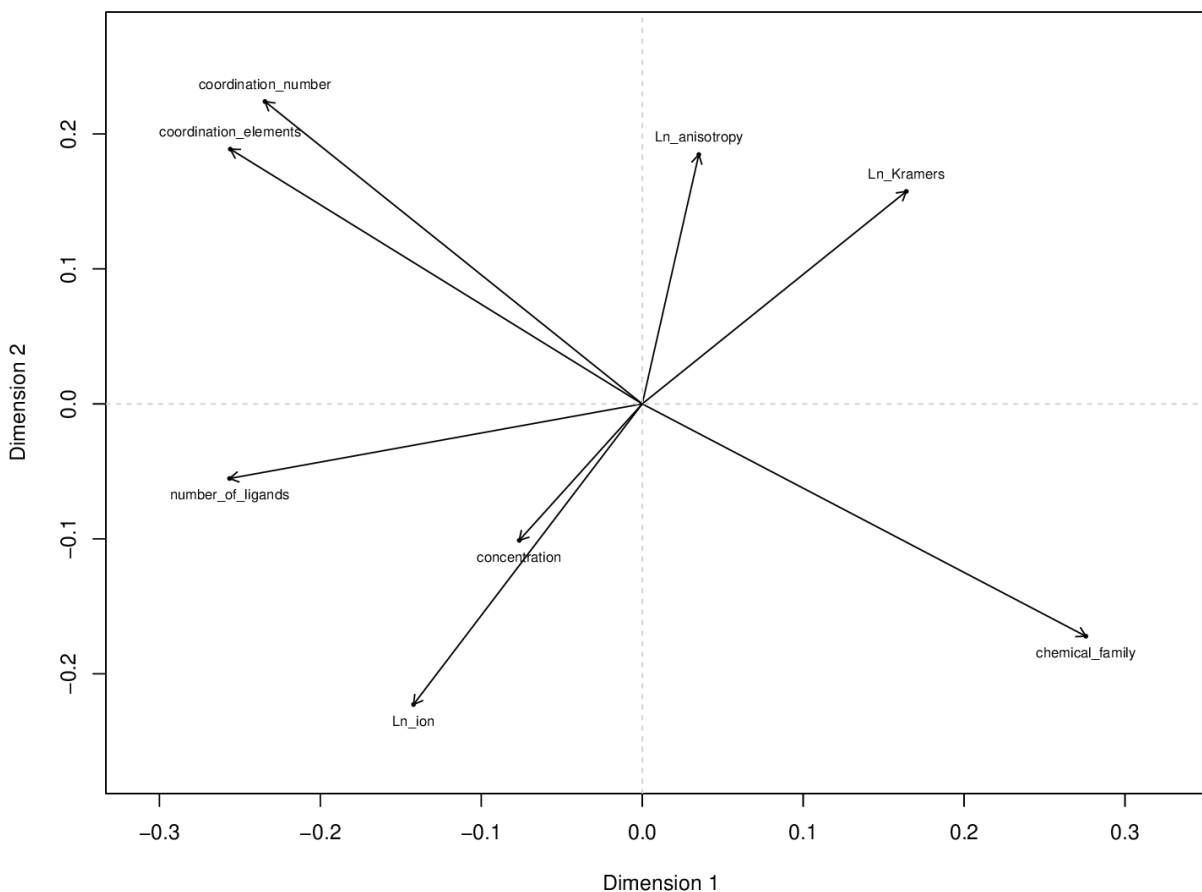
All qualitative results presented in this section considered the whole dataset containing data from literature from 2003 to 2019 for the analyses of chemical variables that follow. Additionally, we repeated the study with the data subset in the timeframe 2003-2017 (~1000 samples instead of ~1400), and the conclusions were robust, with no difference resulting from whether one considers the whole data set from 2003-2019 or only 2003-2017 subset. All quantitative numbers given herein are also consistent between the two studies, within a 5% difference. We can therefore conclude that the relations among the chemical variables are stable, *i.e.* no new trend has been revealed since 2017.

4.1. Initial multiple correspondence analysis

Here we are striving to determine the existing statistical correlations among the chemical variables in the studied sample. This is necessary in order to avoid being misled later on by meaningless correlations between chemical design variables and physical behaviour. For example, we find that the variables “number of ligands” and “coordination elements” happen to be strongly correlated with each other, then it is likely that they will both display the same correlations with a given physical behaviour. In particular, one can expect that an “all-nitrogen coordination environment” will be strongly correlated with “number of ligands = 2”, and with “chemical family = LnPc₂”, and relatively few other complexes in the dataset present only nitrogens as donor atoms. Therefore, if one obtains a correlation between a desirable physical behavior and “chemical family = LnPc₂”, it would be unwarranted to deduce that this behavior can be obtained solely by employing an all-nitrogen coordination environment, or solely by preparing complexes with 2 ligands.

Correspondence Analysis (CA) or reciprocal averaging is a multivariate statistical technique that is employed for the graphical analysis of the dependence or independence of a set of categorical variables from data in a contingency table. It consists in summing up the information in the rows and columns so that it can be projected on a reduced subspace, and represent simultaneously the row and the column data, allowing to obtain conclusions about each pair of variables.

CA only requires data to be organized in categories. Since in our case there are more than two variables, we employed Multiple Correspondence Analysis (MCA). Different approaches for MCA have been proposed; we employed the widely used Gifi system.⁵³ This system consists of a set of multivariate methods developed around the Alternating Least Squares (ALS) algorithm. Among these methods, Homogeneity Analysis provides a model that is equivalent to MCA. ALS's solution for Homogeneity Analysis is known as HOMALS. We employed the R homals package to obtain the following graphical representations.⁵⁴ Results are plotted in Supplementary Figs. 14, 15 and 16.



Supplementary Figure 14 | Multiple Correspondence Analysis: minimal representation of each of the variable loadings on the two main dimensions.

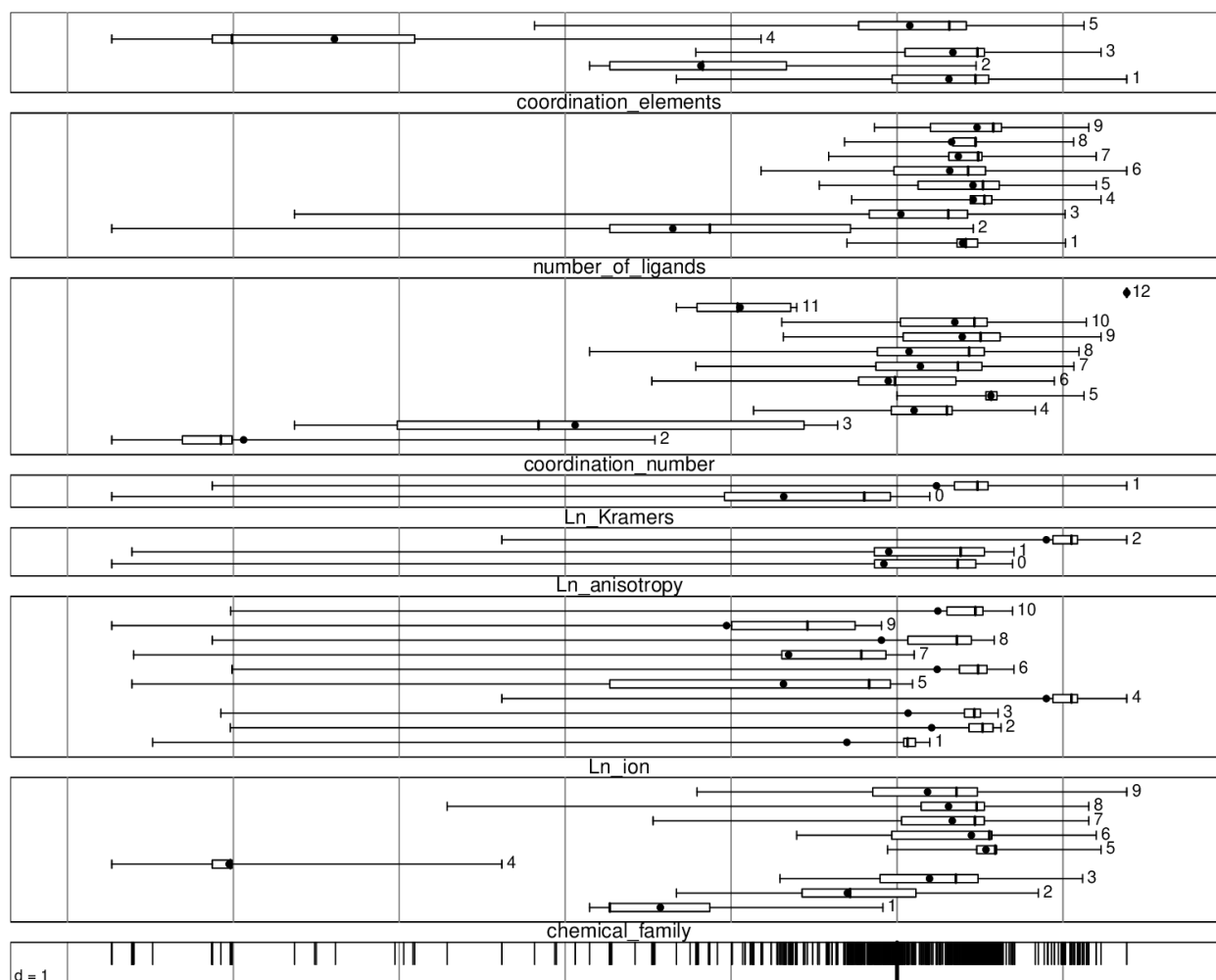
The graph in Supplementary Fig. 14 is read as follows: (i) the length of the vector approximates the variation within each variable, (ii) the cosine between two vectors approximates the correlation between two variables, *i.e.* parallel vectors correspond to perfectly correlated variables, (iii) the distance between the endpoints of two vectors approximates the dissimilarity between the two variables, (iv) the projection of each vector allows to order the data points for that variable. These two MCA dimensions will be employed to understand further analysis, in particular clustering studies. Supplementary Figures 15 and 16 are complementary to Supplementary Fig. 14, and allow for a more complete understanding.

We employed the R ade4 package⁵⁵ for MCA, which only allows the analysis of categorical variables, and obtained the results collected in Supplementary Table 1 for the correlation ratio of each variable.

Supplementary Table 1 | Correlation ratio of each chemical variable with the two MCA dimensions.

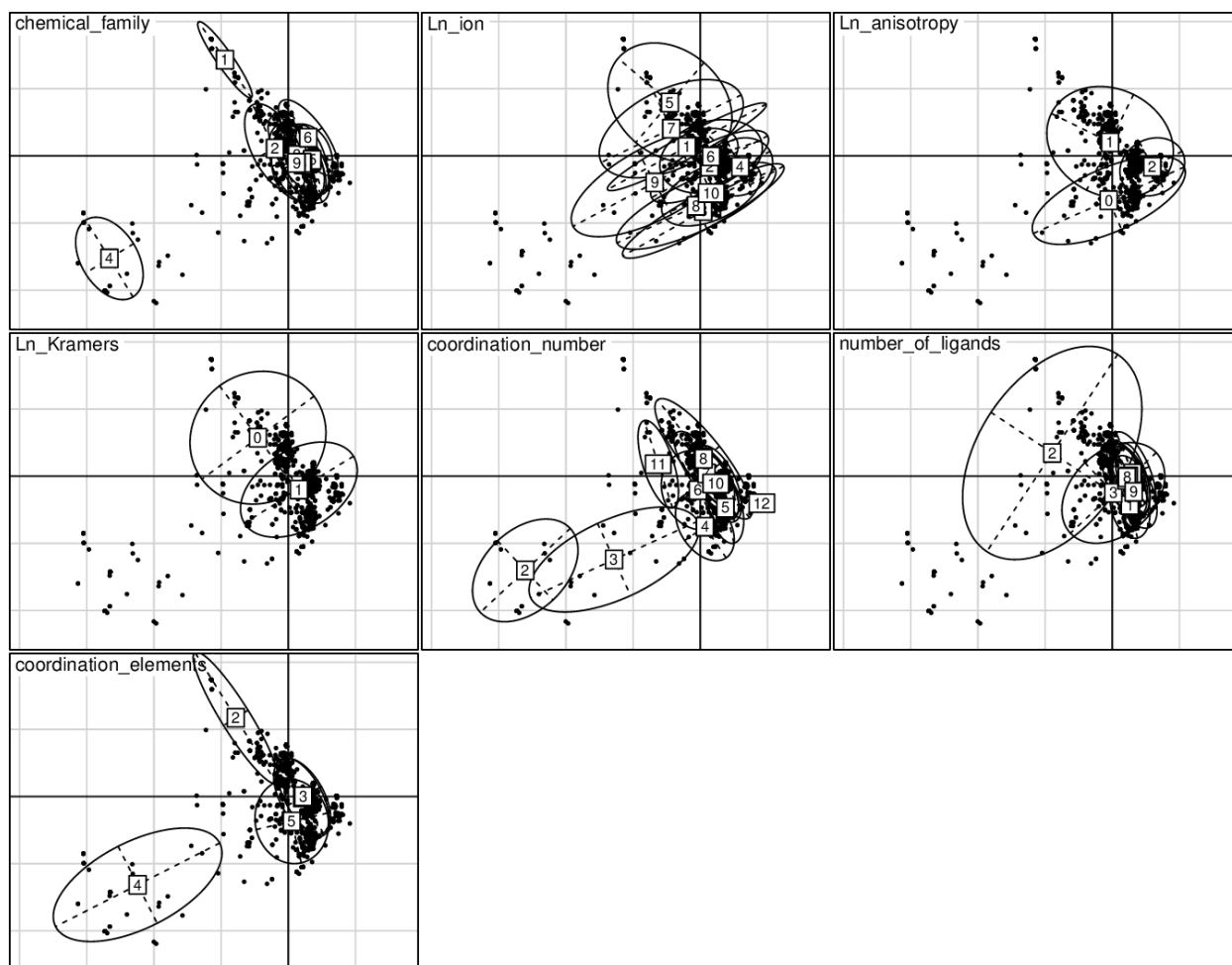
	RS1	RS2
chemical_family	0.81096423	0.6147058
Ln_ion	0.20607706	0.5364464
Ln_anisotropy	0.05097696	0.3121107
Ln_Kramers	0.16243450	0.2918366
coordination_number	0.62057925	0.3528815
number_of_ligands	0.47815893	0.1020615
coordination_elements	0.73301849	0.5353323

To achieve some clarity in the following data-rich representations, we assigned numerical labels to all categorical values as indicated in Supplementary Section 1. Employing these labels and within the same package we obtained the following complementary boxplot representation (Supplementary Fig. 15) that allows us to see the distribution of values, for each variable, along the axis defined by the MCA dimension 1. It is easy to see that the most extreme negative values of MCA dimension 1 are displayed by samples that have carbon or nitrogen as coordination elements, 2 ligands, CN = 2 or 3, as well as those of the metallocene chemical family. As significant positive values in MCA dimension 1, one needs to highlight Gd^{3+} , as well as isotropic complexes which are obviously the same ones.



Supplementary Figure 15 | Boxplots for the distribution along the first MCA dimension of the different categorical values for the chemical variables. See the numbering convention for the categories of the variables in Supplementary Section 1.

A further alternative representation, depicting the distribution of values for the different variables in the dataset as subsets of points was also done (Supplementary Fig. 16). This allows to locate the different values for each chemical variable in terms of positive and negative value ranges for the MC dimensions 1 and 2 simultaneously. At the same time, it allows us to observe overlap between chemical variables, *e.g.* CN = 2 or 3 are in overlap with the metallocene family and with coordination by carbon. Similarly, there is a significant overlap between the LnPc₂ family, complexes with 2 ligands, Ln = Tb and a coordination sphere formed by nitrogen atoms. As we will see in Supplementary Section 4.2, while this kind information points into a clear direction, specialised representations and statistical studies will allow us to study parameter association by clustering.



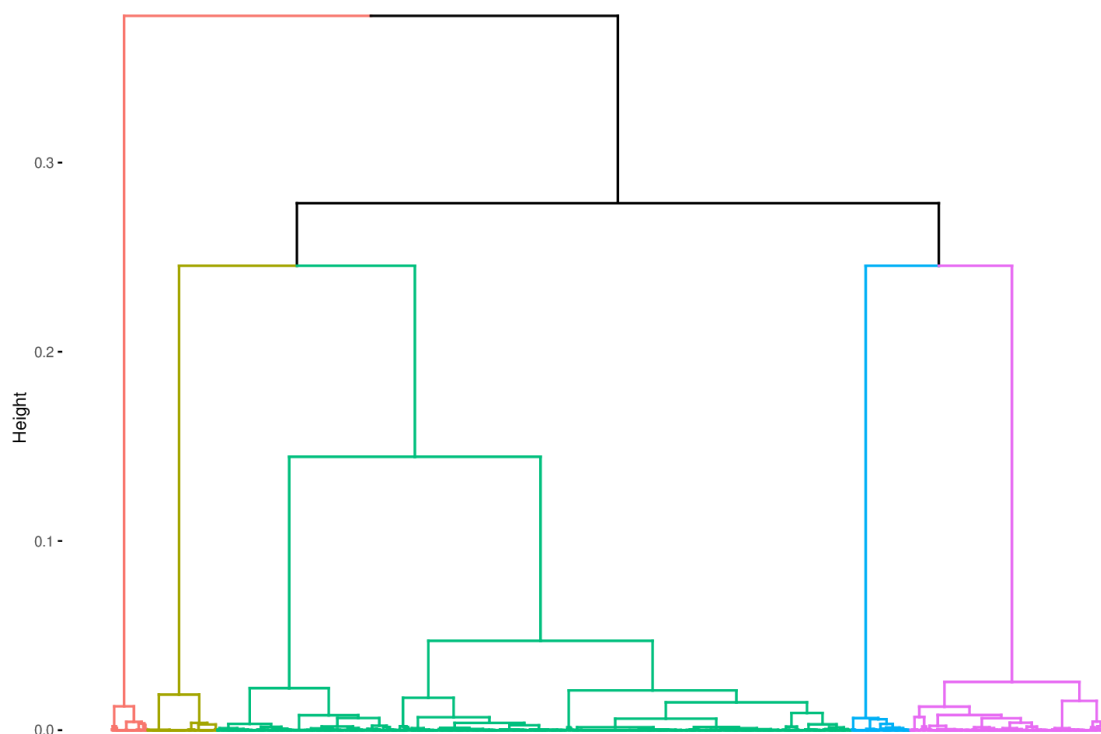
Supplementary Figure 16 | Subsets for the different values of each of the seven categorical chemical variables in the plane of the two MCA dimensions.

4.2. Clustering studies for the chemical variables

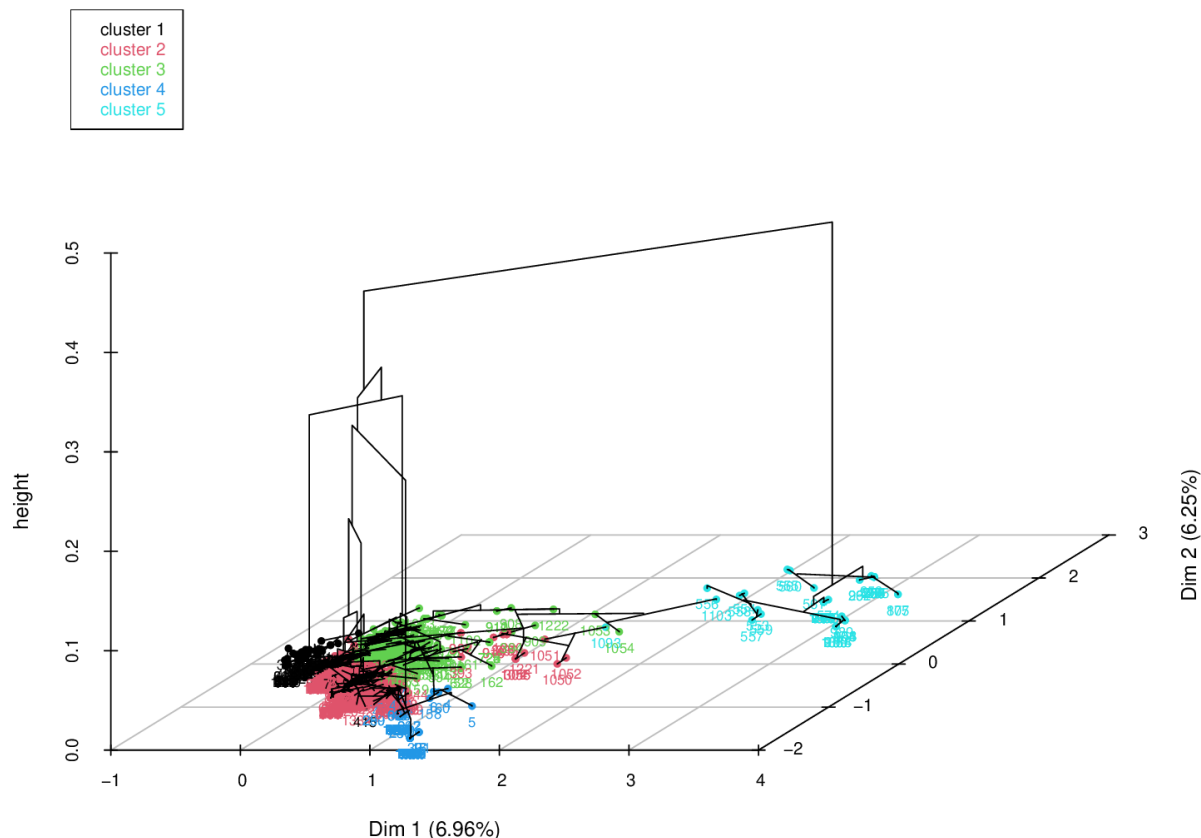
Clustering studies were performed as an independent test. In particular, we employ the package FactoMineR in R to perform the MCA.⁵⁶ This allows a graphical representation of the distances between individual samples and the relations between variables and their values. The goal in this case is to detect within the data types or profiles of data with similar characteristics. In other words, this procedure groups the values for the chemical parameter sets corresponding to individual measurements in families that present an overall similarity.

Due to the nature of our study, this is a crucial step since in practice chemical parameters are not homogeneously distributed as in a purely combinatorial approach. On the contrary, different research groups have chemical expertise in the preparation of different classes of compounds, and often, also evolving ideas on which design strategies would be more relevant for the desired physical property. This means that different research groups at different times focus on different chemical families and strategies for the molecular design of SIMs. As a result, the overall

number of samples (~1400) can be judiciously divided in a small set of hierarchical clusters which share certain common features, as a kind of molecular taxonomy. Again, this will help us put in context our findings: it is to be expected that, when finding a pattern or a magneto-structural trend, we will actually be seeing the behaviour of a cluster rather than the influence of an isolated parameter. Supplementary Figs. 17 and 18 show two different perspectives on the dendrogram resulting from the clustering.



Supplementary Figure 17 | Dendrogram visualization of the calculated hierarchical clustering on the factor map.



Supplementary Figure 18 | Perspective view of the dendrograms visualization of the calculated hierarchical clustering on the factor map.

We found the following 5 tipologies (for details see Supplementary Figs. 19.1 and 19.2):

- Cluster A is small (6% of the samples) and corresponds almost perfectly with the set of Gd^{3+} compounds, or, equivalently, of isotropic complexes. Properties that are strongly overrepresented in this cluster compared to the whole sample include belonging to the “radical” chemical family, number of ligands = 5 and a coordination sphere formed by oxygen only.

- Cluster B is the largest one (63% of the samples), and is composed entirely of oblate ions. 90% of the total of all Dy^{3+} samples are inside Cluster B, however there is a large minority (33.3%) of samples inside Cluster B which are based on non- Dy^{3+} ions. Cluster B also includes ~75% of all samples of “mixed ligands”, of “other families” and where the coordination sphere is a mixture of Oxygens and Nitrogens, and 70% of the samples where the coordination sphere is all Oxygen.

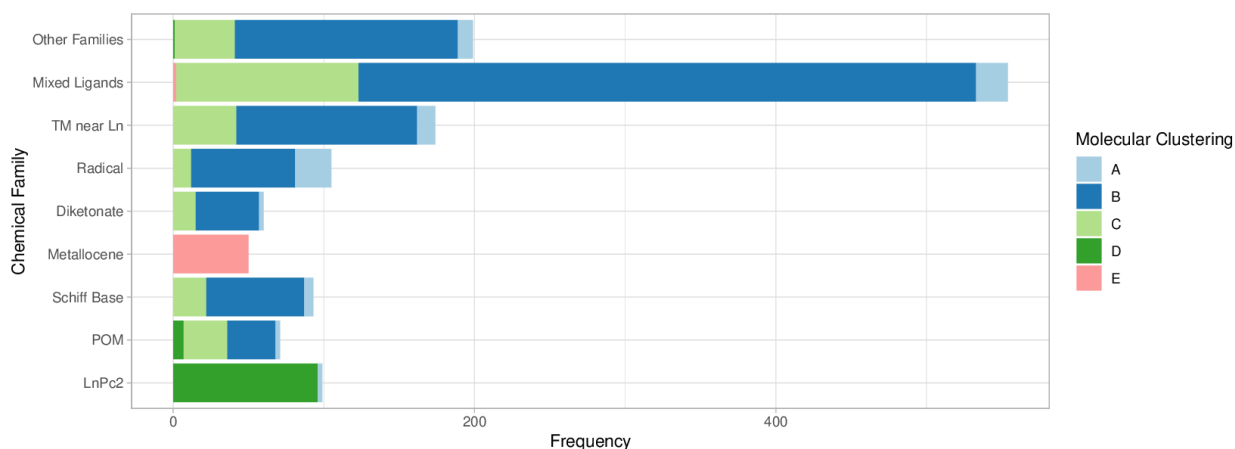
- Cluster C is the second largest one (20% of the samples), and it is composed almost entirely of prolate Kramers ions. Above 50% are Er^{3+} , and almost 30% are Yb^{3+} . Additionally, coordination number = 8 is strongly overrepresented in this cluster.

- Cluster D is small (7.4% of the samples), includes practically all Pc double-deckers ($LnPc_2$), and indeed corresponds very well with this chemical family. The match is weaker in the case of the categories corresponding to all Nitrogen in the coordination sphere, 2 ligands and 8 atoms in the coordination sphere, in the sense that there is a minority of samples with these features which are

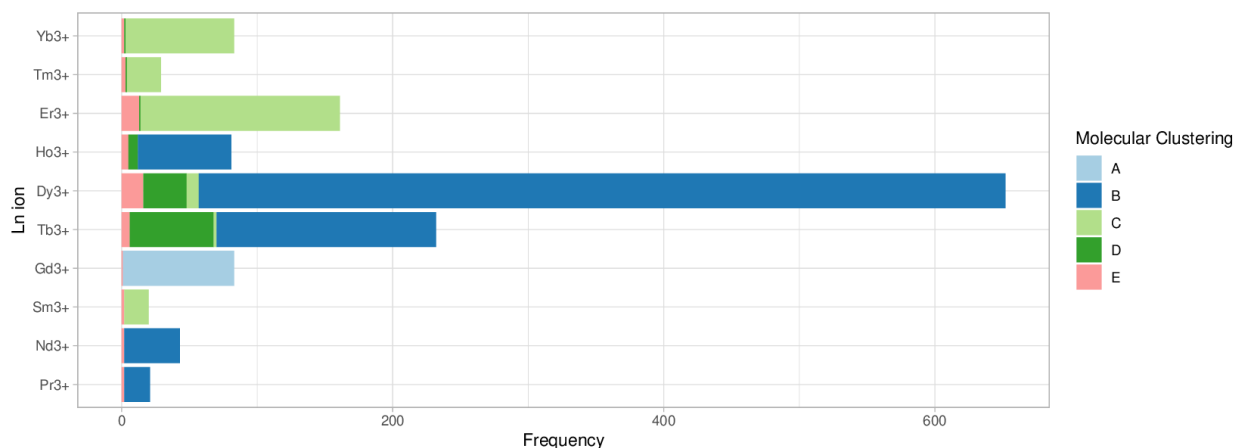
outside this Cluster (Supplementary Fig. 19.2). 60% of the samples in Cluster D are based on Tb^{3+} , 30% are based on Dy^{3+} .

-Cluster E, which is the smallest (3.7% of the samples), corresponds almost perfectly to the metallocene family and, like in Cluster D, the match with all-Carbon coordination, coordination number = 2, and number of ligands = 2 is weaker since some samples with these features are outside this cluster. The samples in Cluster E are more often based on prolate than oblate ions (~40% prolate), but significantly less so than in the total set (~20% prolate). This can be related with the fact that, while ~30% of samples in Cluster D are based on Dy^{3+} , this is much less than for the total dataset (~50% Dy).

a

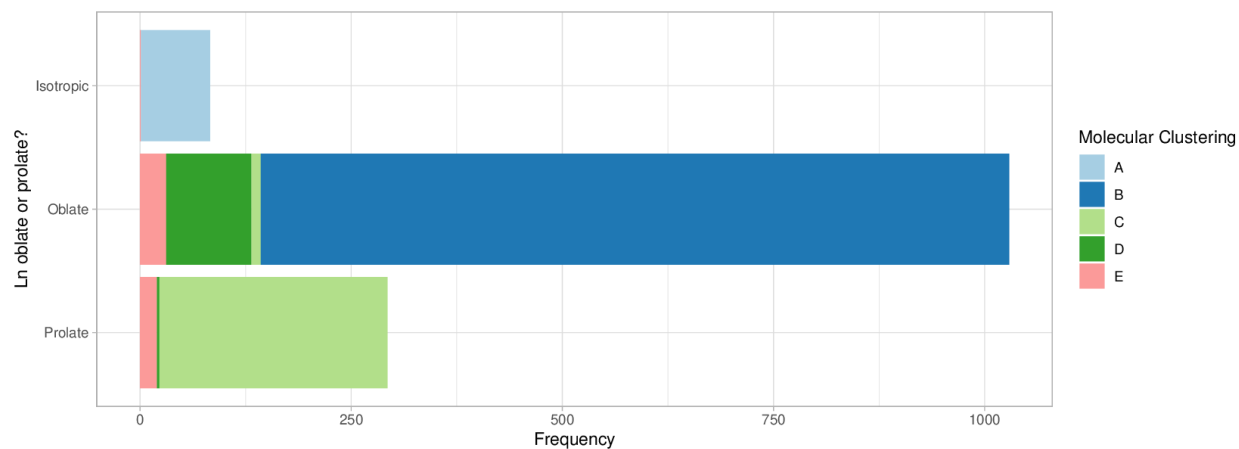
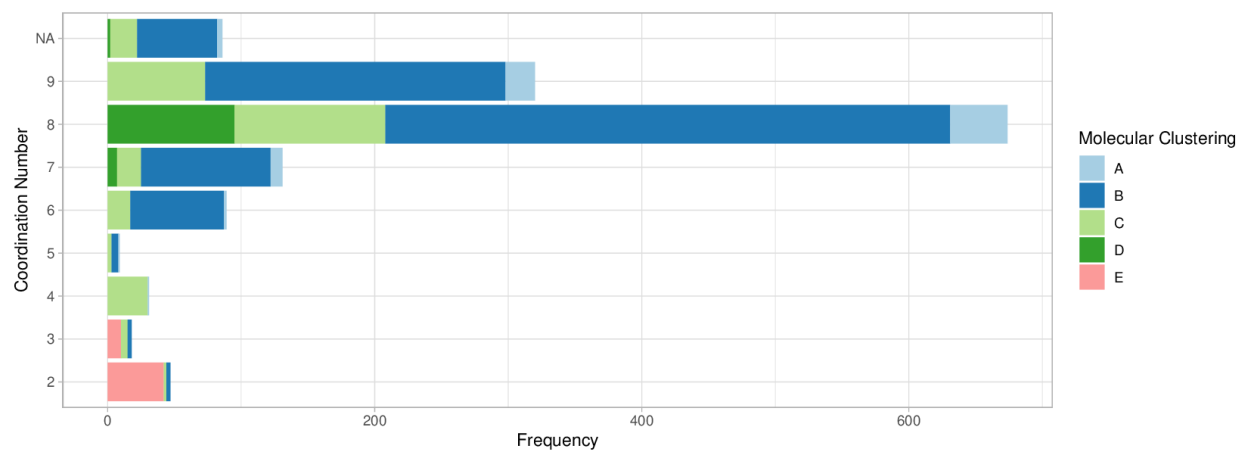
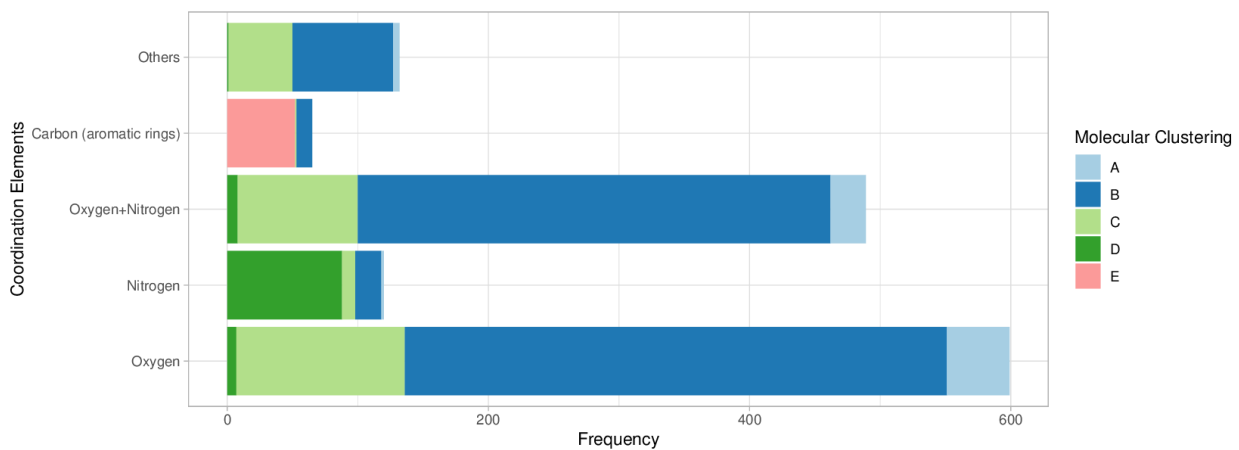


b



Supplementary Figure 19.1 | Bar charts representing the frequencies of chemical variables, filled according to the molecular clustering described in this section. a, chemical families, b, Ln ions.

Note that the dataset downloadable from the SIMDAVIS dashboard includes an alternate lower cut to the same hierarchical clustering mol_cluster_2, finding up to 7 distinct molecular clusters.

a**b****c**

Supplementary Figure 19.2 | Bar charts representing the frequencies of chemical variables, filled according to the molecular clustering described in this section. a, oblate vs prolate nature of the ion, b, coordination numbers, c, coordination elements.

4.3. Lognormal modelling

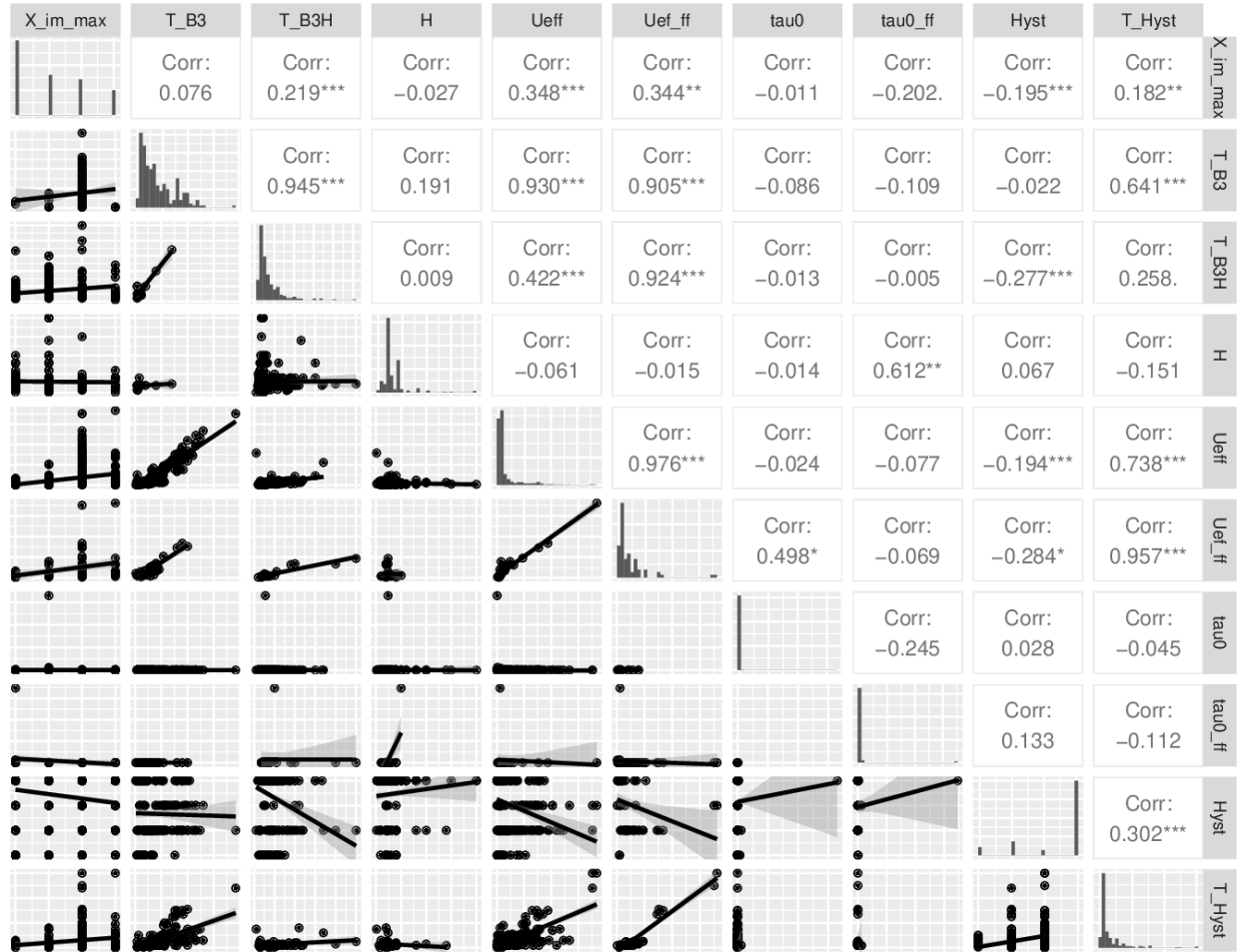
Finally, we applied a lognormal model to detect possible association between variables. The different factors within the model indicate the different associations between the studied variables and parameters. This model works with the frequencies of each variable in the crosstabulation. These frequencies result from each combination of variables, so Poisson's distribution was employed. For any modelization one needs to declare the link function: a function of the expected value of the dependent variable, taking the form of a linear combination of the independent variables. For lognormal modelling, we do not distinguish between dependent and independent variables, since one is rather interested in associations between variables, but one does have a link function which unites the average frequency with the linear predictor, which in this case is the logarithmic function. Within the chemical variables we have many categorical ones, with many levels each. To avoid a useless complication of the analysis, we start by studying the relation between the lanthanide ion, its anisotropy and spin parity (Kramers or not). This serves solely as a test for the modelling and the integrity of our data, since we know that these are associated beforehand: for every lanthanide ion, its anisotropy type and Kramers nature is well defined, with no exceptions. As expected, our model found that it is sufficient to work with the lanthanide ion, and we discarded the other two variables for the subsequent clustering studies. We proceeded to use lognormal models, introducing the rest of the chemical variables, one by one, together with the lanthanide ion. We found that the chemical family, lanthanide ion and coordination elements are the main variables and sufficient to reasonably explain the frequencies of the rest of the variables.

Supplementary Section 5. Statistical analysis of the physical variables

For all the statistical analyses of the physical variables that follow in Supplementary Sections 5.1 and 5.3, additionally to the analyses performed for the complete dataset (data from years 2003-2019), we repeated the study with the data subset in the timeframe 2003-2017 (~1000 samples instead of ~1400). All qualitative results presented here are robust whether one considers the whole dataset 2003-2019 or the 2003-2017 subset. Each of the weak numerical correlations indicated in Supplementary Fig. 20 are stable within a 0.2 window, and in particular all correlations higher than 0.9 are stable with deviations within 0.05 window between both subsets. All values for the Akaike Information Criterion (AIC) in Supplementary Tables 2, 3, 4 are higher on average by about a factor of 1.5-2, as expected, since they are roughly proportional to the number of samples.⁵⁷ We can therefore conclude that the quantitative and qualitative relations among the physical variables are stable, *i.e.* no new significant trends have been revealed recently.

5.1. Overview of the main statistical relationships

Here, our goal is to identify statistical relationships among the physical variables. At first, we want to confirm whether the simple model parameters U_{eff} , $U_{\text{eff},2}$, τ_0 are good statistical predictors (*i.e.* present a high correlation with) of the experimental behavior. In particular, whether they are good predictors of T_{B3} , T_{B3H} , T_{hyst} , H , $\chi_{\text{im,max}}$ and “Hyst”. Next, we want to determine whether the predictive power is different between U_{eff} vs $U_{\text{eff,ff}}$, and τ_0 vs $\tau_{0,\text{ff}}$. Supplementary Fig. 20 represents graphically all physical variables, with their relationships in pairs; $U_{\text{eff},2}$ was eliminated from the graph since the scarcity of data produced errors in the correlation test.



Supplementary Figure 20 | Statistical relationships among the physical variables. The diagonal shows the frequency of each value (range) for each of the physical variables. Below the diagonal we see graphical representations to visually show the relation between every pair of variables, and above the diagonal we find the quantification of each correlation, in the case of numerical variables, or an alternate boxplot, in the case of categorical variables.

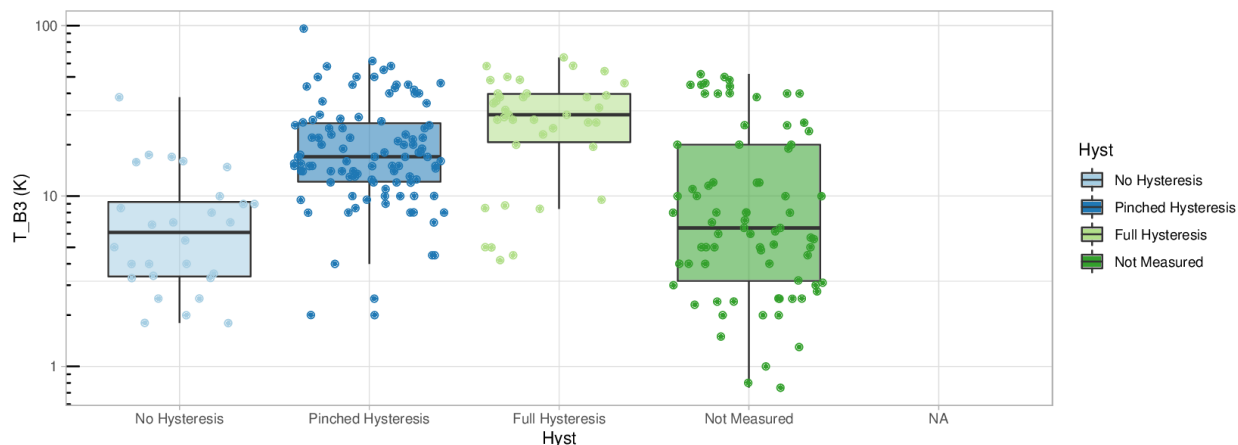
Let us first go over this bidimensional array of statistical representations and analyses, and later on we will focus on the most significant pieces of information.

Keeping in mind the definition of $\chi_{\text{im,max}}$ (Supplementary Section 1), the properties as SIM are better when $\chi_{\text{im,max}}$ takes higher numbers ($0 < 1 < 2$), *e.g.* only the samples with $\chi_{\text{im,max}} = 2$ present values for T_{B3} , while $\chi_{\text{im,max}} = 3$ means having no information. The most frequent value is $\chi_{\text{im,max}} = 0$ (Freq-independent χ''), with the rest being similarly abundant. For T_{B3} and T_{B3H} , higher temperature values are associated with higher values of $\chi_{\text{im,max}}$. Higher effective energy barriers U_{eff} , $U_{\text{eff},2}$, $U_{\text{eff,ff}}$ were estimated for $\chi_{\text{im,max}} = 3$ (corresponding to cases where the SIM properties are not necessarily bad, but just were not characterised via χ'' vs T plots) and especially for $\chi_{\text{im,max}} = 2$ (as expected), compared with systems with worse properties, where almost no difference is found between $\chi_{\text{im,max}} = 0$ and $\chi_{\text{im,max}} = 1$. As in the case of the effective energy barriers, higher hysteresis temperatures T_{hyst} were reported for $\chi_{\text{im,max}} = 3$, and especially for $\chi_{\text{im,max}} = 2$, as expected, compared with systems with worse properties.

The temperatures of the maximum in χ'' at 10^3 Hz are labelled as T_{B3} (when no magnetic field is applied) and T_{B3H} (when a magnetic field H is applied). There are more cases reported in presence of a magnetic field. In both cases, there is a distribution similar to an inverse exponential, meaning higher temperatures are less frequent, but this is more marked for T_{B3H} : when a magnetic field is applied to detect a maximum in χ'' , high temperature values for this maximum are rare. Higher values of the magnetic field H do not correlate with higher values of T_{B3H} . There is a marked difference in the correlations of the temperatures T_{B3} , T_{B3H} with the effective energy barriers U_{eff} , $U_{\text{eff,ff}}$. While there is a very strong correlation between T_{B3} and U_{eff} , for T_{B3H} the correlation only exists for $U_{\text{eff,ff}}$. This is consistent with the presence of other relaxation mechanisms in these cases, such as the QTM, which are quenched in presence of a strong field. In contrast with the effective energy barriers, there are no significant correlations between T_{B3} , T_{B3H} and τ_0 , $\tau_{0,\text{ff}}$. This is initially puzzling, since each pair of effective energy barrier and preexponential time are extracted from a single fit (Supplementary Section 5.3). Finally, there is a systematic qualitative improvement of the hysteretic behaviour with higher values of T_{B3} , T_{B3H} . In other words, high values of T_{B3} , meaning short-term (millisecond) magnetic memory up to a high temperature, are frequently associated with the presence of hysteresis. Moreover, within cases with hysteresis, short-term magnetic memory up to a high temperature is associated with the presence of full hysteresis rather than pinched hysteresis. While this cannot be clearly seen in Fig. 20, it is evident in Fig. 21. In contrast, the quantitative correlation of the hysteretic temperature T_{hyst} with higher values of T_{B3} , T_{B3H} is relatively weak in the case of T_{B3} , and nonexistent for T_{B3H} .

H is the external magnetic field applied to measure T_{B3H} . It presents very weak (and negative) correlations with the effective energy barriers (both U_{eff} and $U_{\text{eff,ff}}$). High values of U_{eff} are visibly correlated with the sample presenting hysteresis ($\text{Hyst} = 1$), and within it, with samples

presenting coercivity ($H_{\text{yst}} = 2$). These correlations are stronger in the case of $U_{\text{eff,ff}}$. The attempt times τ_0 and $\tau_{0,\text{ff}}$ are however very poorly correlated, both with their corresponding barriers and with the other properties. As we will see in Supplementary Section 5.3, this is probably due to the high dispersion in values: at least a qualitative correlation is visible when one works on a logarithmic scale.



Supplementary Figure 21 | Boxplots of T_{B3} grouped by categories of hysteretic behaviour.

5.2. Simple frequency distributions

Let us start by examining the individual frequency distributions of T_{B3} , T_{B3H} , U_{eff} , $U_{\text{eff,ff}}$ and T_{hyst} , *i.e.* the five single-variable bar chart representations of their distribution of values throughout the population (diagonal graphics in Supplementary Fig. 20). In all cases, an initial visual inspection evidences a roughly inverse exponential decay, or perhaps a gaussian distribution centered around very small values. This can be interpreted as a mostly random distribution of values, a signal that the studied population is large and mostly unbiased. An interesting exception can be found in T_{B3} , which takes a bimodal distribution. This has different possible interpretations, but likely just means that a fraction of the research in the field was focused on types of compounds where the median of T_{B3} is at or above the maximum values of the other chemical families, *i.e.* the LnPc_2 family, see Supplementary Fig. 11.1, where it can be compared with the much less marked difference in the case of U_{eff} , where the distribution of the LnPc_2 family is less skewed to very high values.

5.3. Correlations between physical variables

As can be seen in Supplementary Fig. 20, the highest correlations involve U_{eff} and $U_{\text{eff,ff}}$. U_{eff} is highly correlated with T_{B3} and with T_{hyst} . $U_{\text{eff,ff}}$ is highly correlated with U_{eff} , T_{B3} and T_{B3H} . Furthermore, we apply Pearson's test to verify the correlation between U_{eff} and $U_{\text{eff,ff}}$. We obtained a very robust correlation between the two variables, with a p-value $< 2.2 \cdot 10^{-16}$, a 95% confidence interval for the correlation of 0.951-0.989 and an estimated correlation of 0.976. The

same procedure is applied to U_{eff} and $U_{\text{eff},2}$, obtaining results that are robust but substantially less so: p-value $< 1.113 \cdot 10^{-7}$, with a 95% confidence interval for the correlation of 0.701-0.941 and an estimated correlation of 0.864.

We apply the Akaike Information Criterion (AIC), a well-established method that evaluates how well a statistical model fits the data it was generated from. This method allows to compare the quality of a series of candidate models using the same data, so that the AIC estimates the quality of each of the models relative to the others. As the models are used to represent the process that generated the data, this representation will be losing some information because of the flaws of the model, and the AIC estimates the relative amount of information lost by each candidate model. This means, the preferred model will have the lowest AIC value in a given set of candidate models. To implement AIC, we employ the R functions `lm`, `glm` with family = binomial (stats package from R base)⁵⁸, and `multinom` (nnet package).⁵⁹ The results can be found in Supplementary Tables 2, 3 and 4.

Supplementary Table 2 | AIC modelling experimental physical (response) variables as a function of modelling variables U_{eff} , $U_{\text{eff},2}$, τ_0 .

Response variable	Data points	Variables included in the model	Significant variable	AIC
χ''_{max}	23	$U_{\text{eff}}, U_{\text{eff},2}, \tau_0$	-	55.04
		$U_{\text{eff}}, U_{\text{eff},2}$	-	49.04
		U_{eff}, τ_0	-	65.52
		$U_{\text{eff},2}, \tau_0$	-	55.62
T_{B3}	4	-	-	-
T_{B3H}	14	$U_{\text{eff}}, U_{\text{eff},2}, \tau_0$	τ_0	2.64
		$U_{\text{eff}}, U_{\text{eff},2}$	-	35.35
		U_{eff}, τ_0	τ_0	0.98
		$U_{\text{eff},2}, \tau_0$	τ_0	4.25
		τ_0	τ_0	2.27
Hyst	23	$U_{\text{eff}}, U_{\text{eff},2}, \tau_0$	-	44.49
		$U_{\text{eff}}, U_{\text{eff},2}$	-	40.49
		U_{eff}, τ_0	-	40.56
		U_{eff}	-	36.56
		$U_{\text{eff},2}, \tau_0$	-	43.13
T_{hyst}	4	-	-	-

Supplementary Table 2 contains the analysis based on the modelling variables U_{eff} , $U_{\text{eff},2}$ and τ_0 . The analysis quantifies the models employing these three variables to explain the different response variables: $\{\chi''_{\text{max}}, T_{\text{B3}}, T_{\text{B3H}}, \text{Hyst}, T_{\text{hyst}}\}$. The results are heterogeneous. Depending on

the response variable chosen, the best modelling variables can be either $\{U_{\text{eff}}, U_{\text{eff},2}\}$, or τ_0 , or U_{eff} . Since very few samples are modelled considering two independent barriers $(U_{\text{eff}}, U_{\text{eff},2})$, the data are scarce and the results are not statistically significant.

Supplementary Table 3 | AIC modelling experimental physical (response) variables as a function of modelling variables U_{eff} , τ_0 .

Response variable	Data points	Variables included in the model	Significant variable	AIC
χ''_{max}	608	U_{eff}, τ_0	-	1381.05
		U_{eff}	-	1378.16
		τ_0	-	1542.43
T_{B3}	186	U_{eff}, τ_0	U_{eff}	693.98
		U_{eff}	U_{eff}	692.98
		τ_0	-	1051.61
T_{B3H}	261	U_{eff}, τ_0	U_{eff}	770.73
		U_{eff}	U_{eff}	768.74
		τ_0	-	818.99
Hyst	601	U_{eff}, τ_0	-	40.56
		U_{eff}	U_{eff}	36.56
		τ_0	-	42.04
T_{hyst}	134	U_{eff}, τ_0	U_{eff}	650.3
		U_{eff}	U_{eff}	648.32
		τ_0	-	780.94

Supplementary Table 3 contains the analysis including U_{eff} and τ_0 , *i.e.* when an Orbach-only model with a single energy barrier is considered, and quantifies the models employing these variables to explain different response variables: $\{\chi''_{\text{max}}, T_{\text{B3}}, T_{\text{B3H}}, \text{Hyst}, T_{\text{hyst}}\}$. The results are very robust in this case. U_{eff} is consistently found to be the significant variable and the one producing the lowest AIC value.

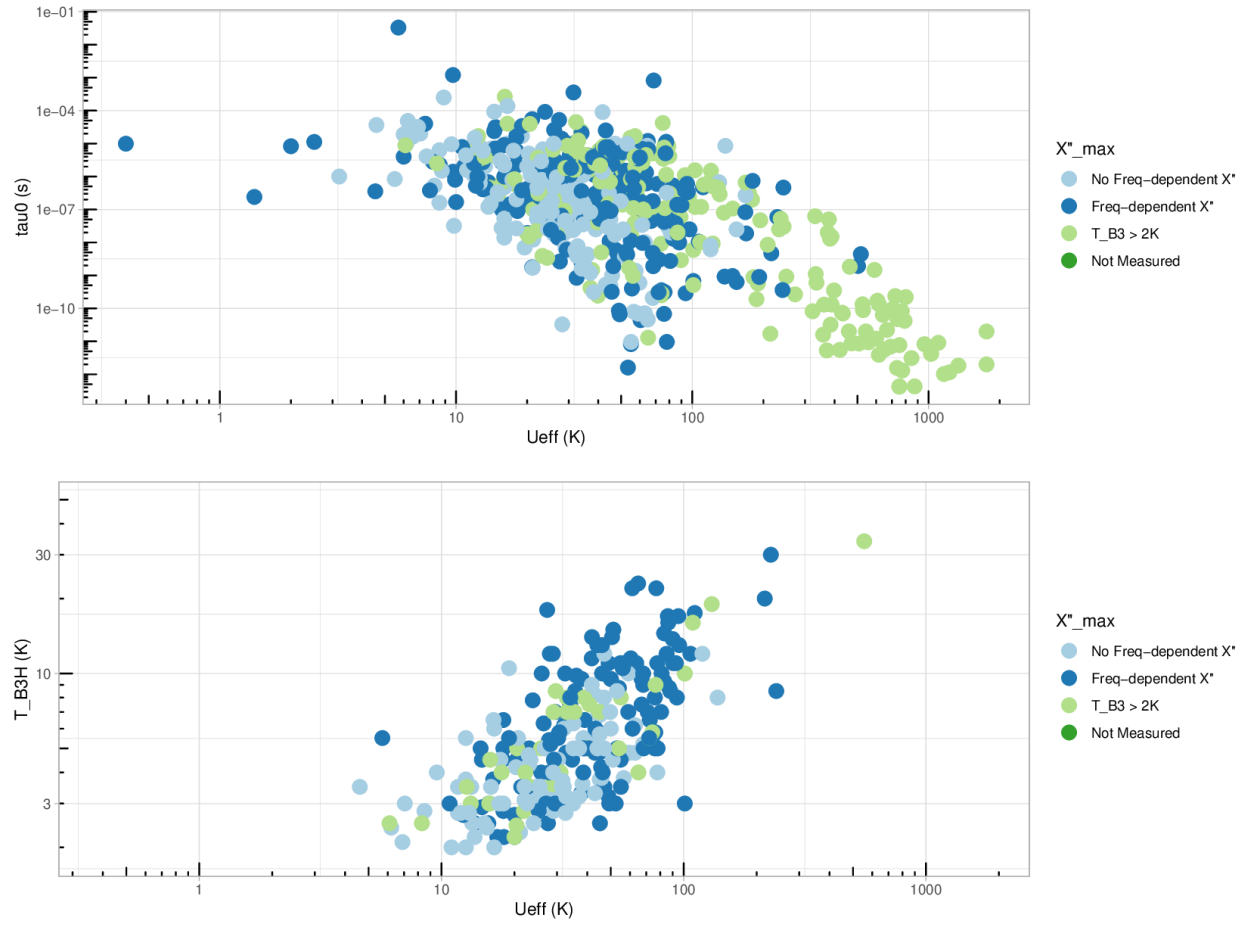
Supplementary Table 4 | AIC modelling experimental physical (response) variables as a function of modelling variables $U_{\text{eff,ff}}$, $\tau_{0,\text{ff}}$.

Response variable	Data points	Variables included in the model	Significant variable	AIC
χ''_{max}	68	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	-	169.58
		$U_{\text{eff,ff}}$	-	165.33
		$\tau_{0,\text{ff}}$	-	185.89
T_{B3}	27	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	88.5
		$U_{\text{eff,ff}}$	$U_{\text{eff,ff}}$	91.51
		$\tau_{0,\text{ff}}$	-	137.25
T_{B3H}	23	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	$U_{\text{eff,ff}}$	74.62
		$U_{\text{eff,ff}}$	$U_{\text{eff,ff}}$	73.54
		$\tau_{0,\text{ff}}$	-	116.81
Hyst	67	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	-	137.57
		$U_{\text{eff,ff}}$	-	131.57
		$\tau_{0,\text{ff}}$	-	156.68
T_{hyst}	36	$U_{\text{eff,ff}}, \tau_{0,\text{ff}}$	$U_{\text{eff,ff}}$	102.08
		$U_{\text{eff,ff}}$	$U_{\text{eff,ff}}$	102.72
		$\tau_{0,\text{ff}}$	-	191.68

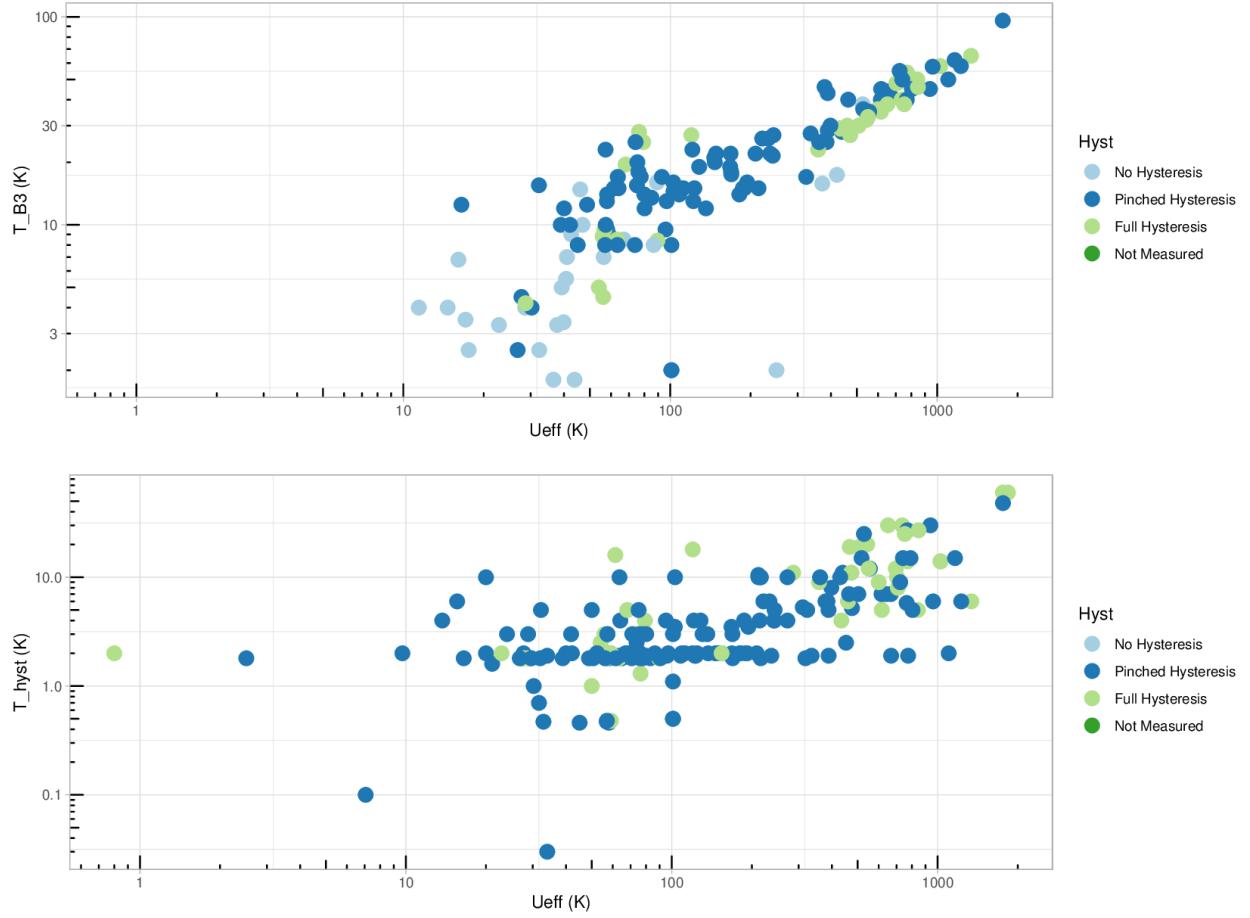
Supplementary Table 4 contains the same analysis but including only $U_{\text{eff,ff}}$ and $\tau_{0,\text{ff}}$, *i.e.* a more complete model that should be closer to reality. The modelling employing $U_{\text{eff,ff}}$ is almost as good as in the case of U_{eff} . However, since information about $U_{\text{eff,ff}}$ is available in less samples, U_{eff} is statistically preferable.

To visualize these correlations, see Supplementary Figs. 22 and 23. The relations between U_{eff} , τ_0 , χ''_{max} , T_{B3H} are represented in Supplementary Fig. 22. Within a wide dispersion, a (log-log) inverse linear relation is apparent between (log-log) U_{eff} and τ_0 (more on this on Supplementary Figs. 24.1 and 24.2) and a (log-log) linear relation is apparent between T_{B3H} and U_{eff} . These graphs also show how samples with higher values of U_{eff} systematically present a maximum in T_{B3} , and in contrast samples where no frequency-dependent χ'' is measured tend to display lower values of U_{eff} . To complete the picture, we represent the relations between U_{eff} , *Hyst*, T_{hyst} , T_{B3} . (Supplementary Fig. 23). A (log-log) linear tendency is apparent when plotting T_{B3} vs U_{eff} ; this is obscured in the case of T_{hyst} vs U_{eff} by the abundance of samples where the hysteresis was characterized only at 2 K. Like in the case of the ac susceptibility, there is a large dispersion of behaviours by samples with longer magnetic memory, in this case meaning the ones presenting whole hysteresis, tend to be grouped around higher values of U_{eff} , with samples presenting no

hysteresis tend to present lower values of U_{eff} and samples with pinched hysteresis presenting typically intermediate values.



Supplementary Figure 22 | Scatterplots depicting the relation of U_{eff} with τ_0 , χ''_{max} , T_{B3H} . τ_0 vs U_{eff} , colored by χ''_{max} (up); T_{B3H} vs U_{eff} , colored by χ''_{max} (down).



Supplementary Figure 23 | Scatterplots depicting the relation of U_{eff} with H_{yst} , T_{hyst} , T_{B3} . T_{B3} vs U_{eff} , colored by H_{yst} (top); T_{hyst} vs U_{eff} , colored by H_{yst} (down).

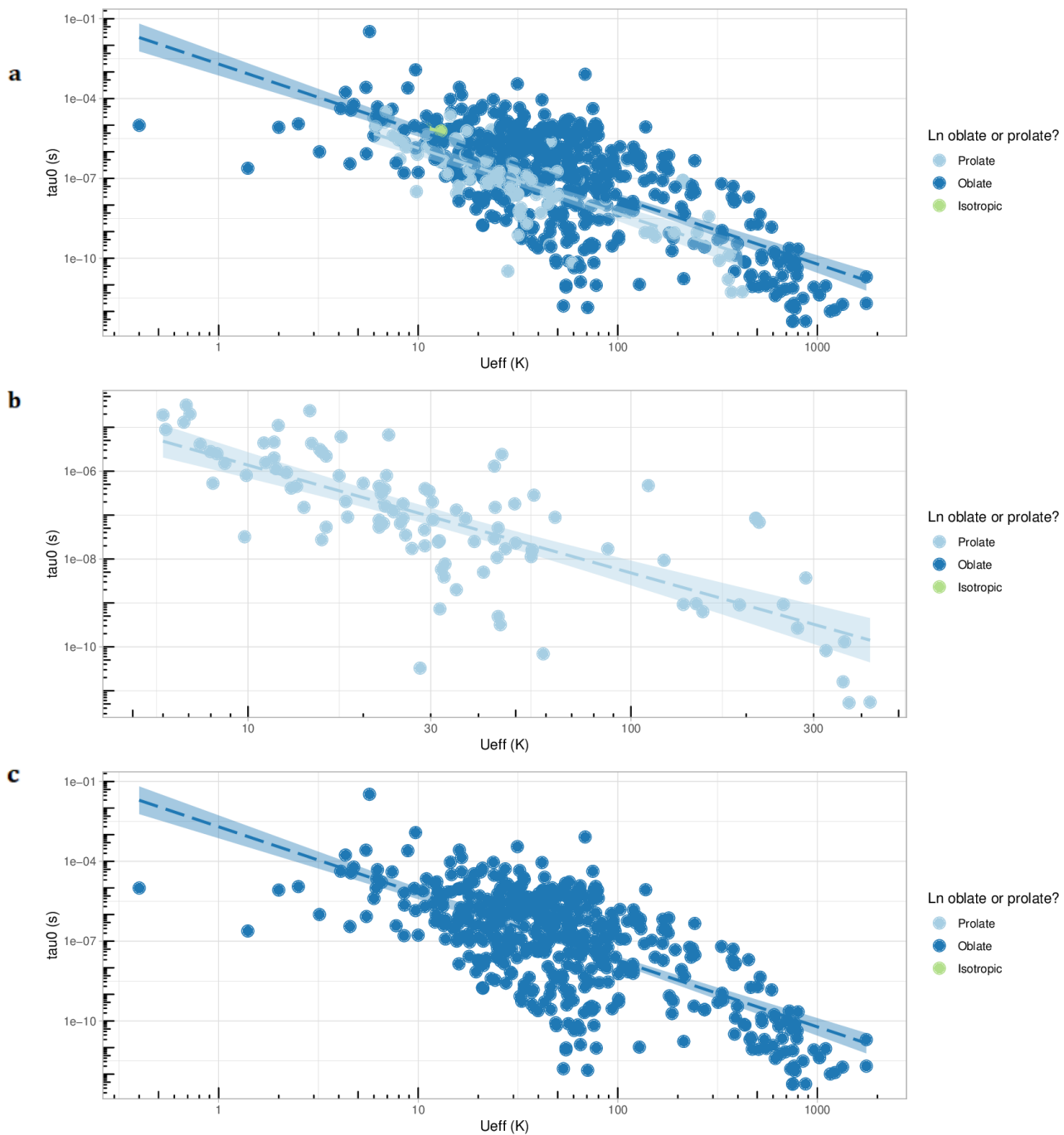
The main conclusion of the study is that U_{eff} derived from a simplistic Arrhenius plot is currently the best single predictor for physical behaviour. This means that, whether we are discussing in terms of the presence of maximum in out-of-phase component of the ac susceptibility (χ''_{max}) or the temperature of said maximum (T_{B3} , T_{B3H}), U_{eff} is a better predictor than τ_0 or $U_{\text{eff},2}$ (note that the number of studies with $U_{\text{eff},2}$ is too small). Also the number of studies deriving $U_{\text{eff,ff}}$ from a full fit considering the other physical processes is very low. Furthermore, the correlation between $U_{\text{eff,ff}}$ and U_{eff} is very high. The combination of the two facts mean that there is no statistical argument for the qualitative observation that $U_{\text{eff,ff}}$ from a full fit is a better predictor for T_{hyst} .

Finally, let us represent the available data in terms of τ_0 vs U_{eff} . Note that the slopes are identical but the constant term is higher for oblate ions compared with prolate ions: at a given U_{eff} the expected τ_0 for oblate ions is ten times higher than τ_0 for prolate ions, meaning an equivalent U_{eff} relaxation will be substantially slower in oblate ions (Supplementary Fig. 21.4). Within the two main oblate ions (Dy^{3+} and Tb^{3+}), the slope is slightly higher for Dy^{3+} , meaning a dramatic

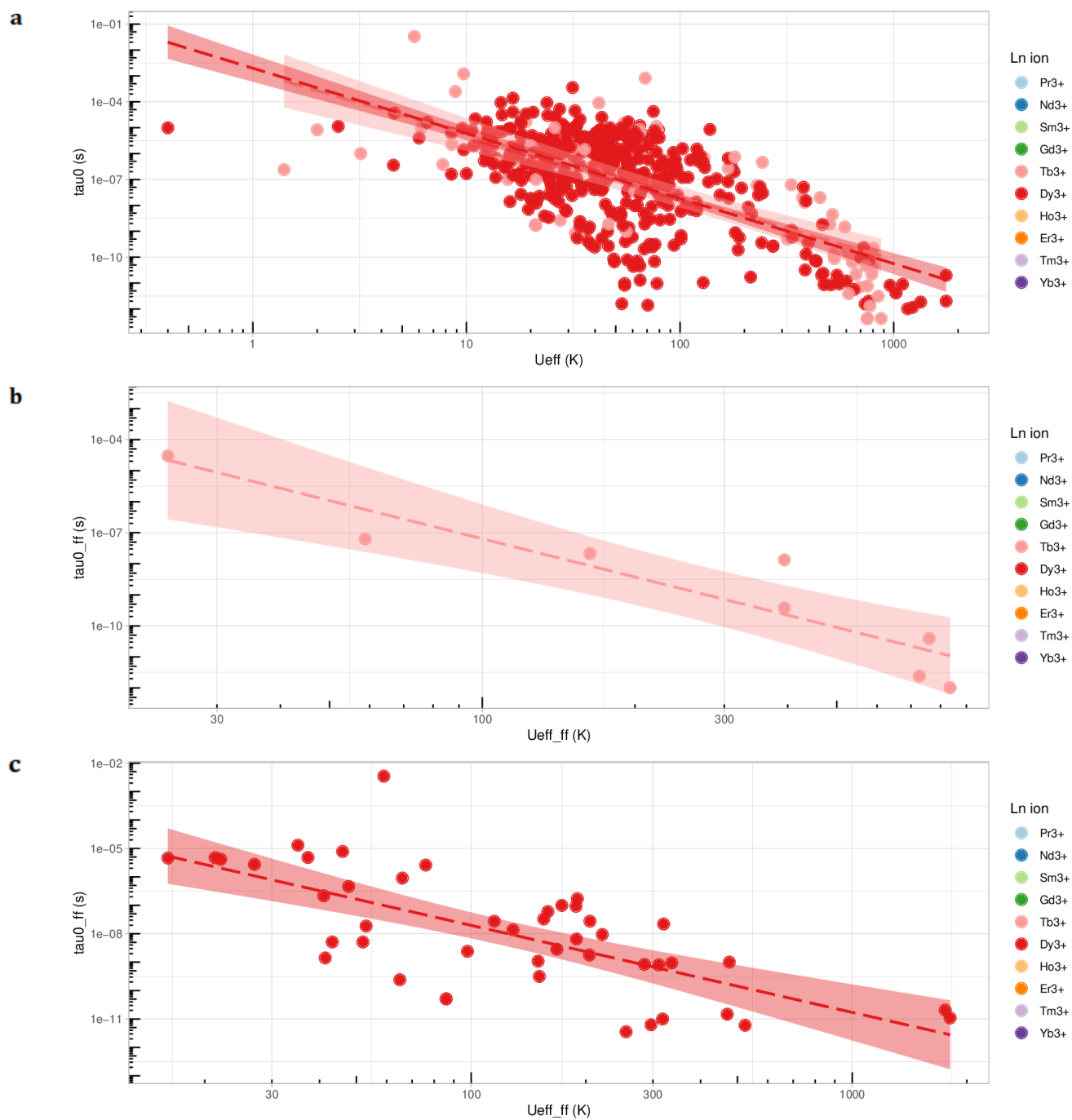
increase in U_{eff} is somewhat more beneficial for Tb^{3+} compared with Dy^{3+} (Supplementary Fig. 21.2).

Supplementary Table 5 | Least squares fits of $\ln(U_{\text{eff}})$ vs $-\ln(\tau_0)$ and $\ln(U_{\text{eff,ff}})$ vs $-\ln(\tau_{0,\text{ff}})$.

Data	Intercept (R_{Or})	Slope (n)
All	839.4	2.437
Prolate	2557.5	2.454
Oblate	504.3	2.506
Tb^{3+}	700.5	2.415
Dy^{3+}	504.0	2.515
Full fit	151.2	2.957



Supplementary Figure 24.1 τ_0 vs U_{eff} , for prolate and oblate ions. a, Comparison between both. b, Only prolate ions. c, Only oblate ions.



Supplementary Figure 24.2 | τ_0 vs U_{eff} and $\tau_{0,ff}$ vs $U_{eff,ff}$ for Tb³⁺ and Dy³⁺. a, Comparison between both. b, Only Tb³⁺ complexes. c, Only Dy³⁺ complexes.

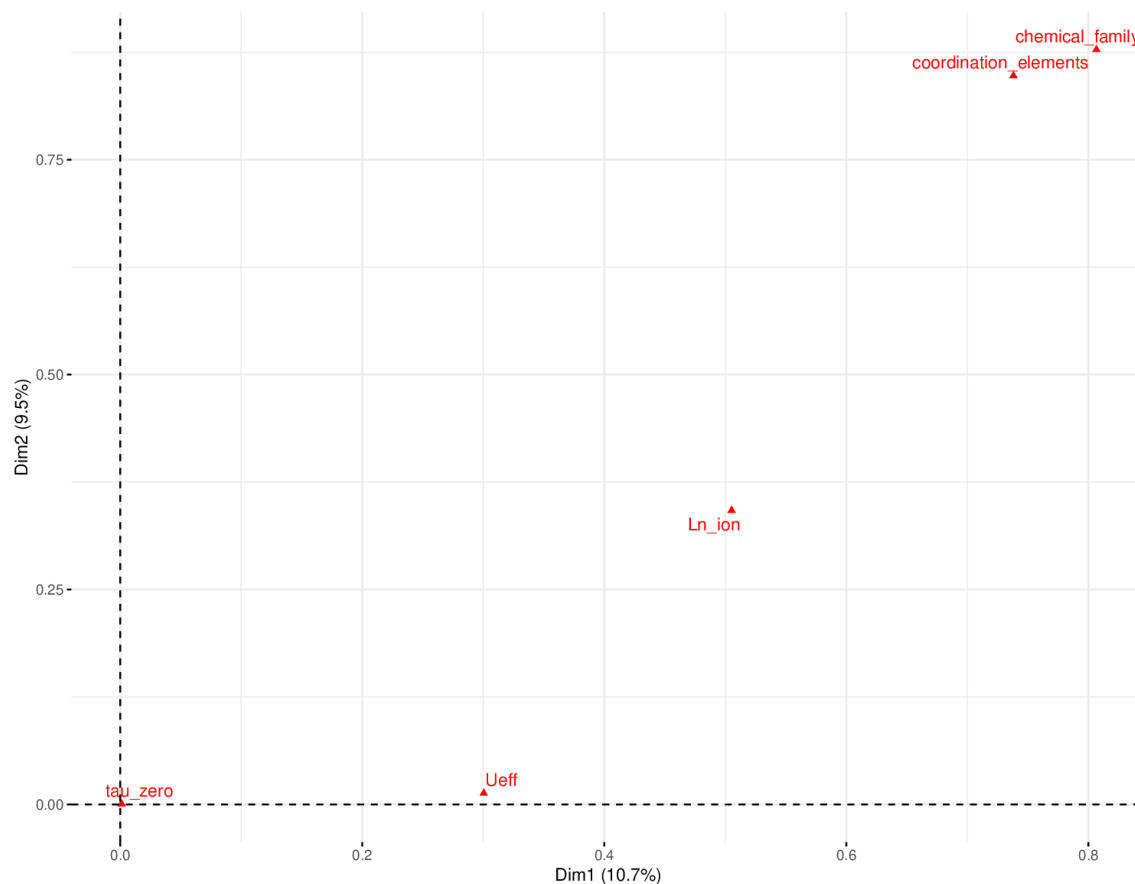
Supplementary Section 6. FAMD and magnetostructural clustering

For all the statistical studies of the physical variables that follow in Supplementary Section 6, we performed the analysis two times, to check for consistency and robustness of the results. In particular, we performed the analysis of the full dataset (~1400 samples) and repeated it independently employing only the data subset in the timeframe 2003-2017 (~1000 samples). We found that all major qualitative results presented here are robust and independently obtained whether one considers the whole set 2003-2019 or the 2003-2017 subset. Furthermore, quantitative data were found to be within a 25% deviation, with a shift towards higher values of U_{eff} , T_{B3} and T_{hyst} in the 2003-2019 set when compared with the 2003-2017 subset.

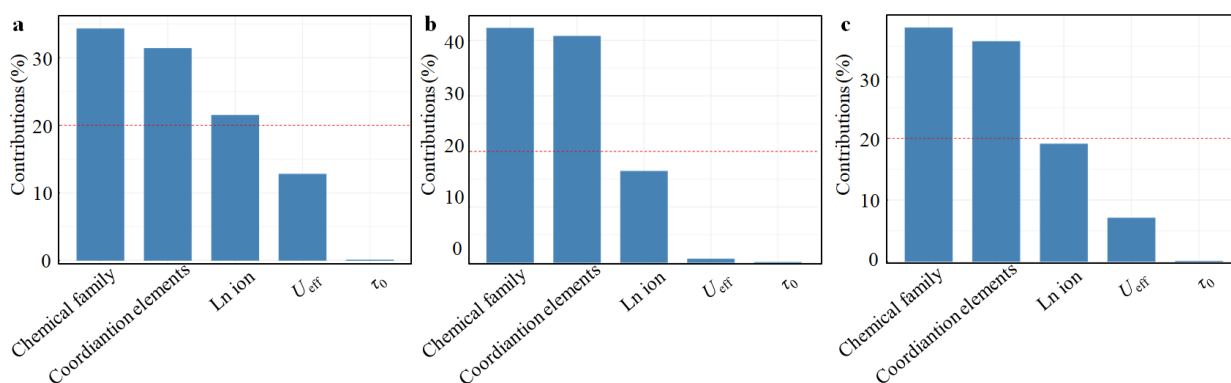
Factorial analysis of mixed data (FAMD) is a factorial method appropriate to analyse data containing both quantitative and qualitative variables. FAMD is a versatile method that acts as Principal Component Analysis for quantitative variables, and as Multiple Correspondence Analysis for qualitative variables. Qualitative and quantitative variables are normalized during the analysis to equilibrate the influence of each in the variable set. In this case this allows us a simultaneous analysis of physical and chemical properties, to perform a hierarchical clustering of samples with the goal of producing a magnetostructural taxonomy in our Ln-based SIMs catalogue. By grouping the samples by taking into consideration their molecular structure and their magnetic behaviour, we can aspire to obtain information on the main relation between form and function. To perform this analysis and data representation we employed R packages FactoMineR⁵⁶ and factoextra.⁶⁰

We found that the chemical family, the lanthanide ion and the coordination elements are the best chemical predictors, as U_{eff} among the physical parameters. Only 608 samples in the dataset contain quantitative U_{eff} and τ_0 data. We initially worked just with these 608 samples, and later repeated the analysis with all samples, obtaining the same result.

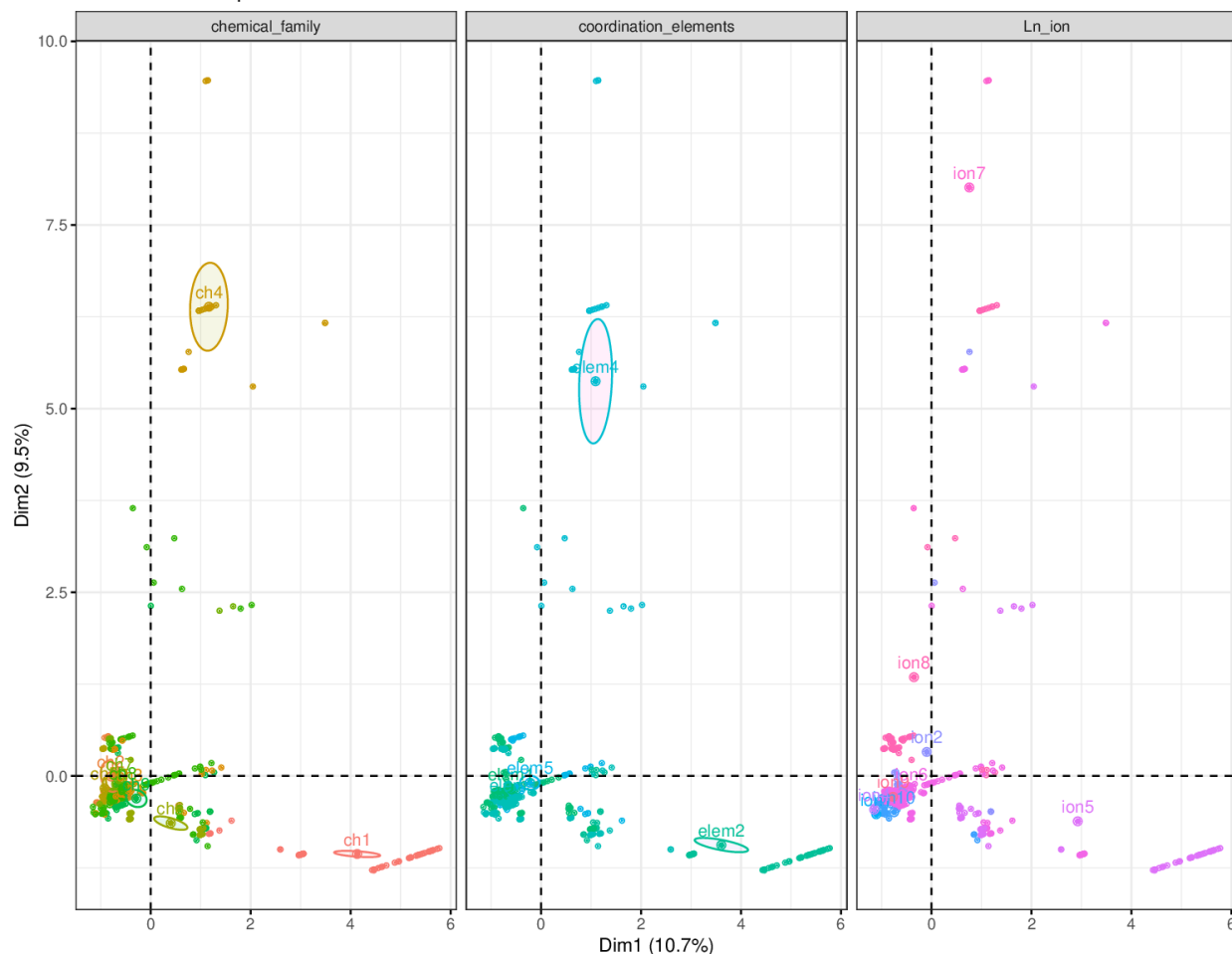
Let us start with representing the relation between the two main FAMD dimensions and the main physical and chemical variables (Supplementary Figs. 25, 26 and 27). Analyzing the contribution from the main chemical and physical variables to the main FAMD dimensions (Supplementary Figs. 25 and 26), one can see that the distinctive traits for both dimension 1 and dimension 2 are the variables “chemical family” and “coordination elements”, with the “Ln ion” choice appears in a distant third place, while “ U_{eff} ” participates only in dimension 1. This is similar to what was seen in Supplementary Section 4.2. The FAMD factor map (Supplementary Fig. 27) provides additional information on the actual values of the variables presented by the samples and their relation to the two main dimensions.



Supplementary Figure 25 | Representation of the physical and chemical variables according to a FAMD method.



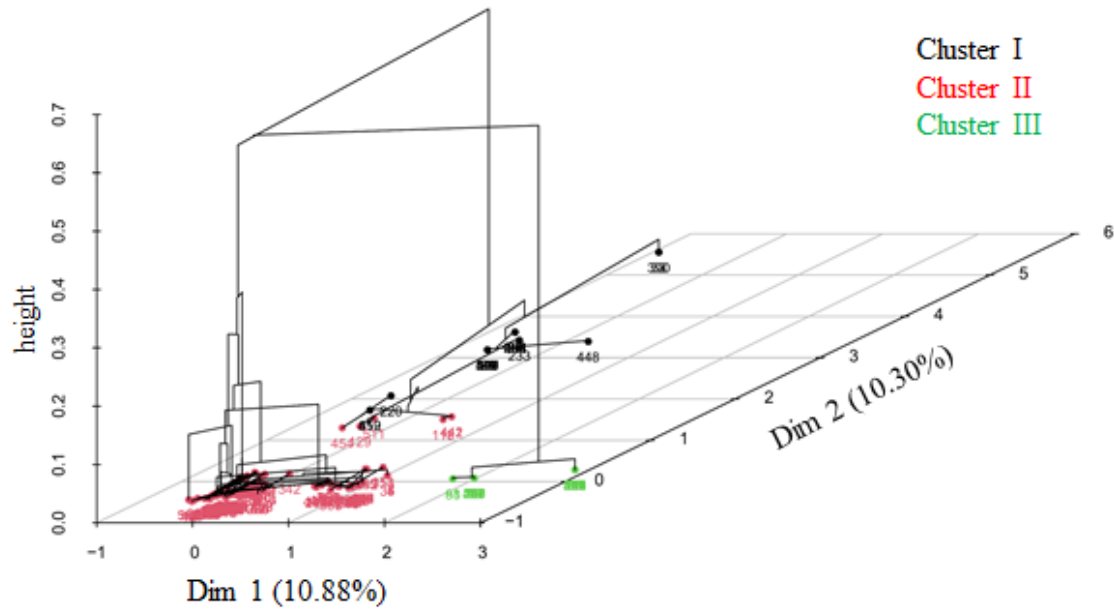
Supplementary Figure 26 | Contribution from the main chemical and physical variables to the main FAMD dimensions. a, Contributions to the dimension 1. b, Contributions to dimension 2. c, Combined contributions to dimensions 1 and 2.



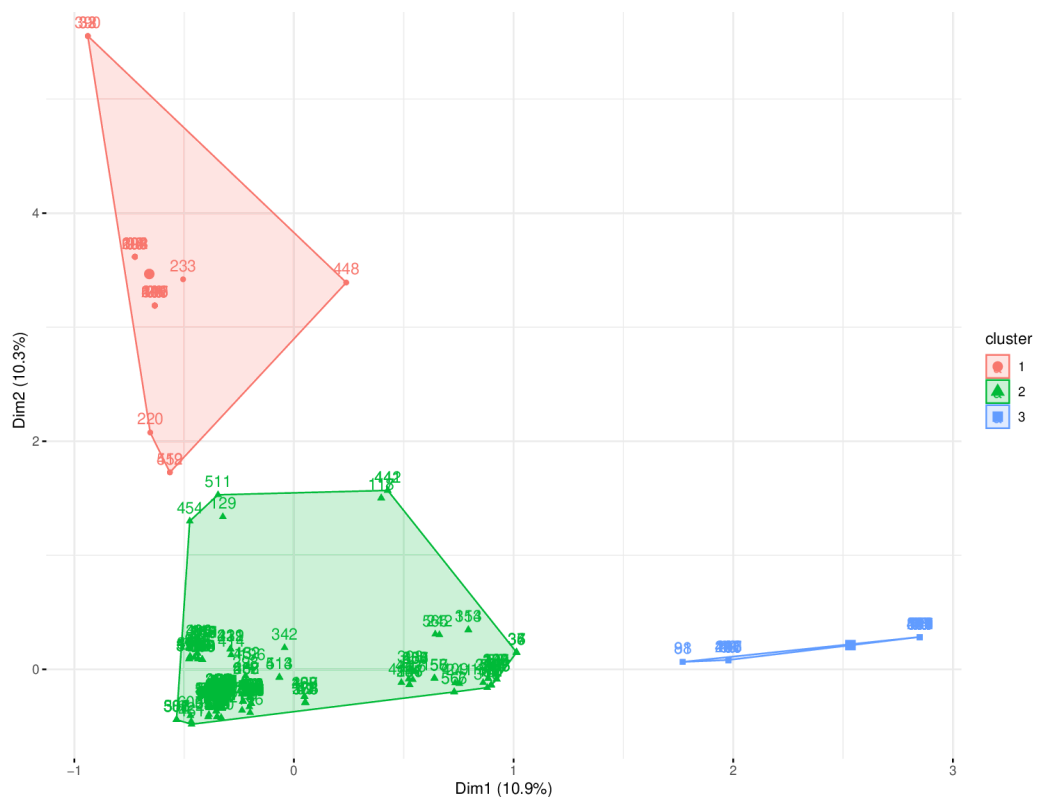
Supplementary Figure 27 | FAMD factor map. The groupings of the different values for the three main chemical variables is shown. See numbering convention for the categories of variables in Supplementary Section 1.

6.1. Magnetostructural clusters

We proceed to analyze the magnetostructural hierarchical clustering. This is comparable with the molecular clustering presented in Supplementary Section 4.2, but considering both physical and chemical variables. Dendrograms are represented in Supplementary Figs. 28 and 29, and a description of the different clusters follows.



Supplementary Figure 28 | Dendrogram depicting the hierarchical clustering on the factor map. The numbers in the plot represent sample_IDs.



Supplementary Figure 29 | Alternate view of the calculated hierarchical clustering on the factor map. The numbers in the plot represent sample_IDs.

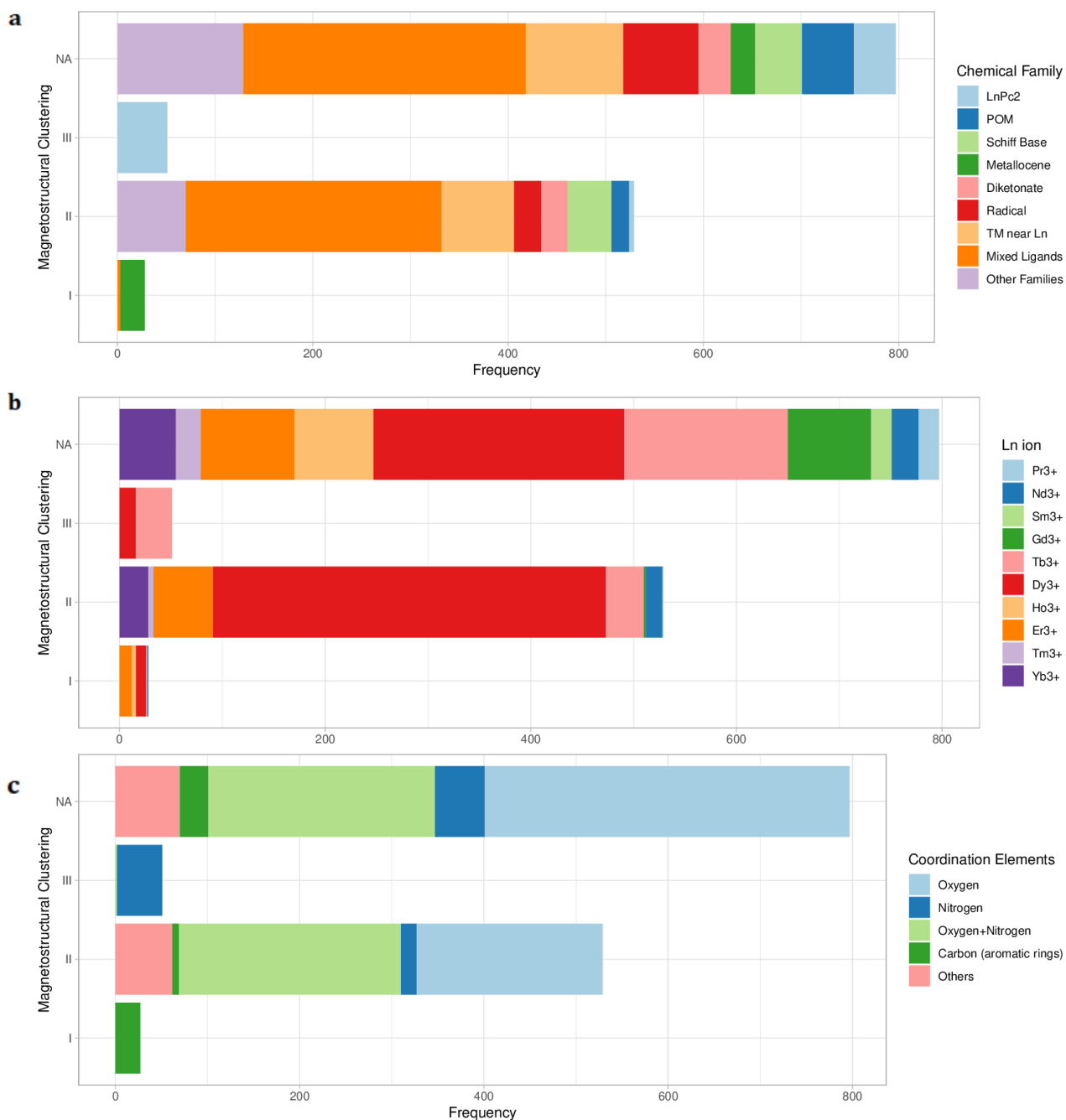
The main results from these analysis are as follows:

- Cluster I: U_{eff} is the most associated variable in cluster I. The average value of U_{eff} (252 K) in cluster I is considerably higher than the general average of U_{eff} (117 K). In addition, the average value of T_{hyst} in cluster I (9.9 K) is also significantly above the average value of T_{hyst} (5.5 K). Indeed, cluster I is characterised by higher-than-average values of U_{eff} and T_{hyst} .
- Cluster II is characterised by close-to-average values of T_{B3} (18.5 K < 19.2 K) and T_{hyst} (5.2 K < 5.5 K), and lower-than average U_{eff} (87 K < 117 K).
- Cluster III, like cluster I but less intensely, is characterised by higher-than-average values for U_{eff} (353 K > 117 K) and T_{B3} (26 K > 19 K).

A partial clustering taking into account of the first 1000 data points (*i.e.* discarding data from 2018 and 2019) results in a very similar classification, but primarily characterizes cluster I by higher-than-average values for U_{eff} and T_{B3} and cluster III by higher-than-average values for T_{hyst} and U_{eff} . As a notable difference, discarding recent data results in a significant decrease in the average value for cluster III down to $U_{\text{eff}} = 199$ K.

This general “magnetostructural” clustering classification, when described strictly from the point of view of the chemical variables, is depicted in Supplementary Fig. 30 and can be simplified to:

- cluster I: metallocene-type sandwiches, carbon as donor atoms, with Ho^{3+} and Er^{3+} as the most abundant ions.
- cluster II: predominantly mixed ligands, *i.e.* a mixture of different coordination ligands, predominantly Dy^{3+} ion, and either only oxygens or a mixture of nitrogen and oxygen as donor atoms. This is by far the most abundant class of compounds with reported U_{eff} .
- cluster III: Tb^{3+} ion (followed by Dy^{3+}), LnPc_2 family, nitrogens as donor atoms. These values for these variables are partially overlapping.



Supplementary Figure 30 | Bar charts for magnetostructural clusters and their relation with the main chemical variables. From top to down, the bar charts are filled according to: **(a)** chemical family, **(b)** lanthanide ion and **(c)** coordination elements in the coordination sphere.

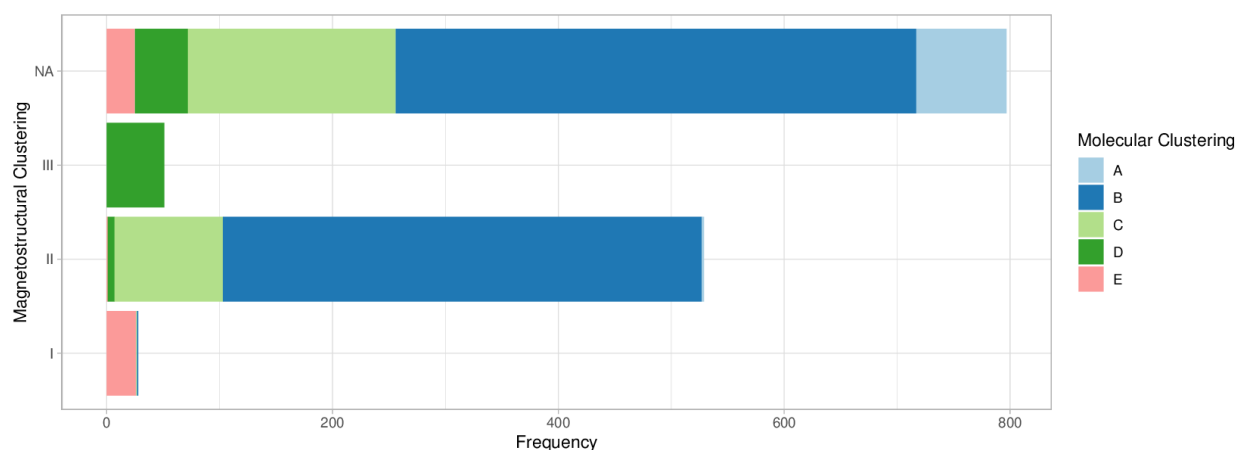
The correlation between the magnetostructural clusters I-II-III and the chemical clusters A-B-C-D-E is depicted in Supplementary Fig. 31, and can be summarized as follows:

-cluster I is mostly composed of samples from cluster E

-cluster II is a mixture of samples from cluster B and C, and as well some from cluster D, but mostly from B

-cluster III is mainly samples of cluster D

-samples outside the I-II-III classification (not assigned), meaning samples with no recorded value of U_{eff} are a mixture of all of the A-B-C-D-E cases, notably including all of the cases of cluster A (Gd^{3+} complexes), and are, in order of relative abundance: B, C, A, D, E.



Supplementary Figure 31 | Bar charts for magnetostructural clusters and their relation with the molecular (chemical) clusters. NA stands for not assigned samples, *i.e.* samples that do not belong in any of the 3 magnetostructural clusters I-III.

Note that the dataset downloadable from the SIMDAVIS dashboard includes an alternate lower cut to the same hierarchical clustering (mag_struct_cluster_2 in the dataset), finding up to 8 distinct magnetostructural clusters.

Supplementary Section 7. Annex: articles included in the study

1. Ishikawa, N., Sugita, M., Ishikawa, T., Koshihara, S. & Kaizu, Y. Lanthanide Double-Decker Complexes Functioning as Magnets at the Single-Molecular Level. *Journal of the American Chemical Society* **125**, 8694–8695 (2003).
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