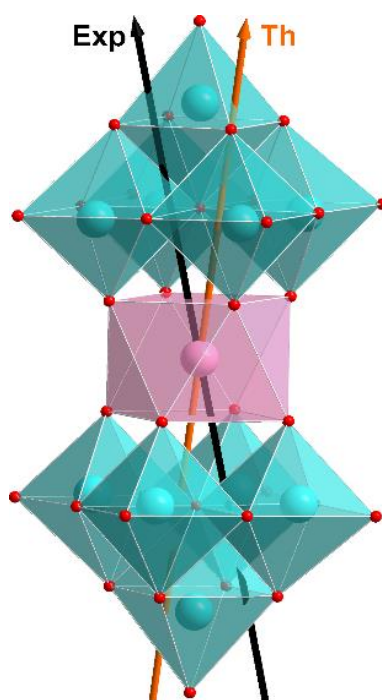


# Chemistry–A European Journal

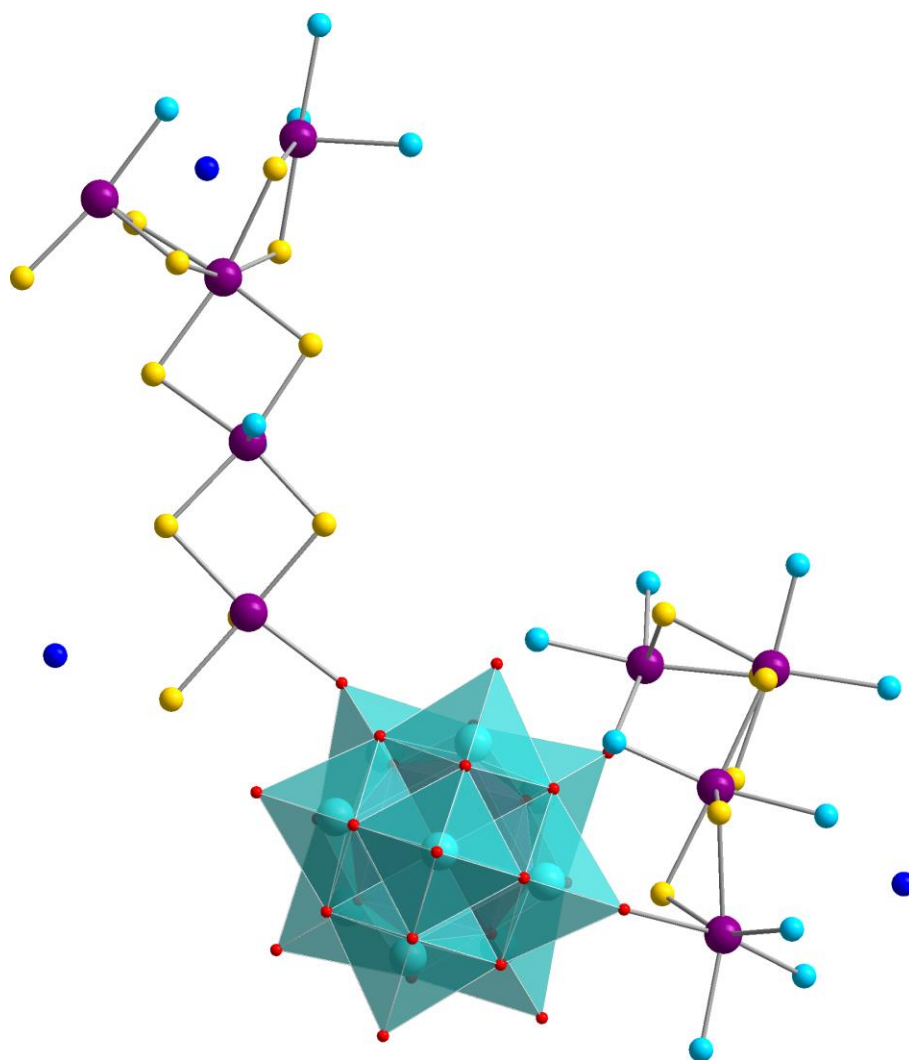
Supporting Information

## **Solvato Modulation of the Magnetic Memory in Isotopically Enriched Erbium Polyoxometalate**

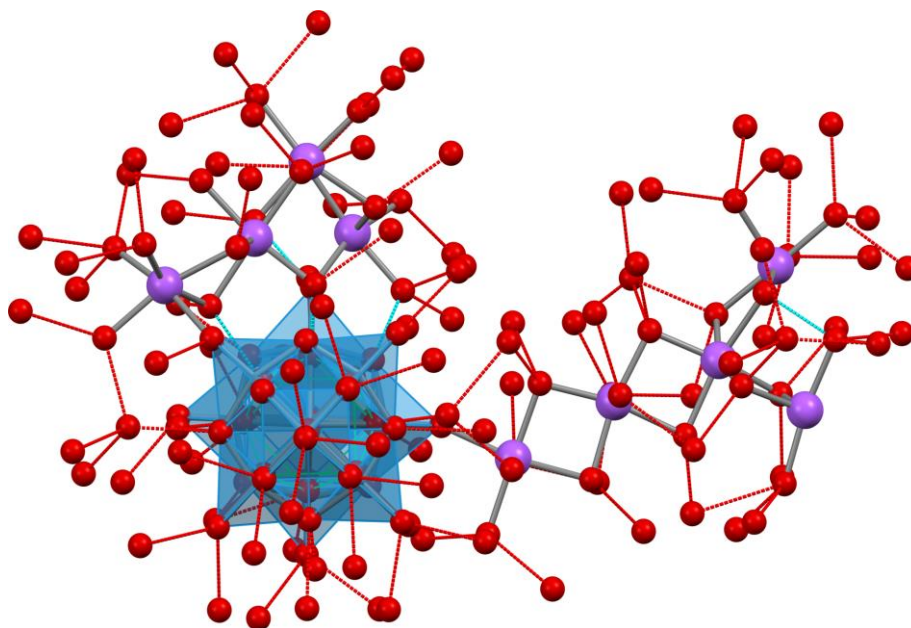
Jessica Flores Gonzalez, Vincent Montigaud, Vincent Dorcet, Kevin Bernot, Boris Le Guennic,\* Fabrice Pointillart,\* and Olivier Cador\*



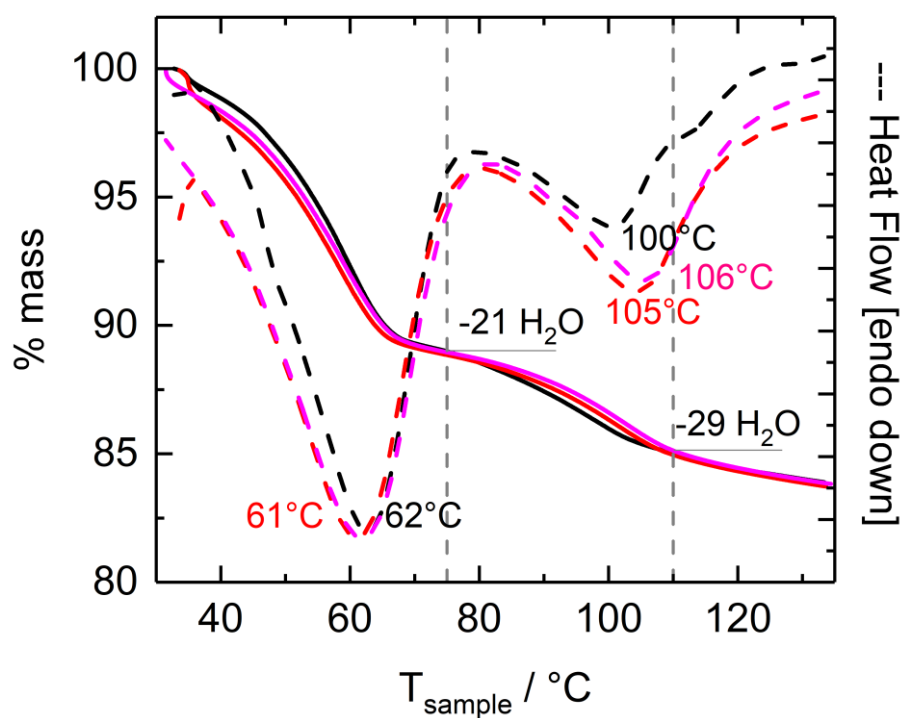
**Figure S1.** Molecular structure of the anionic complex  $[\text{Er}(\text{W}_5\text{O}_{18})_2]^{9-}$  with the representation of the square anti-prism polyhedron around the Er<sup>III</sup> centre (pink) and both experimental (black arrow) and calculated (orange arrow) main anisotropy axis orientation.



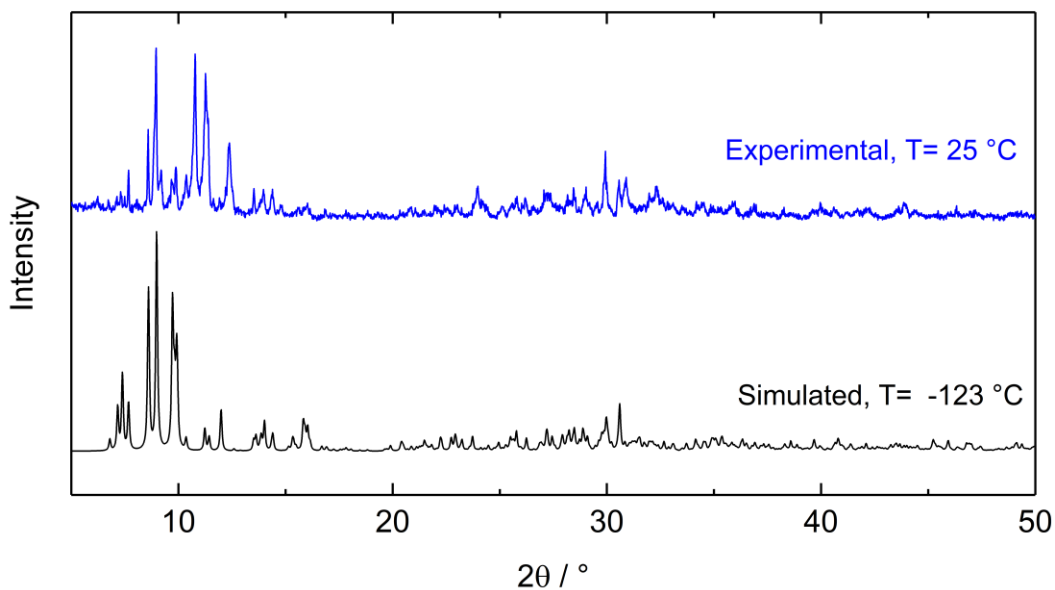
**Figure S2.** View of the asymmetric unit with colour code found in main text expect for water molecules that a drawn with colours depending on their coordination mode: blue (non coordinated), light blue (terminal) and yellow (bridging).



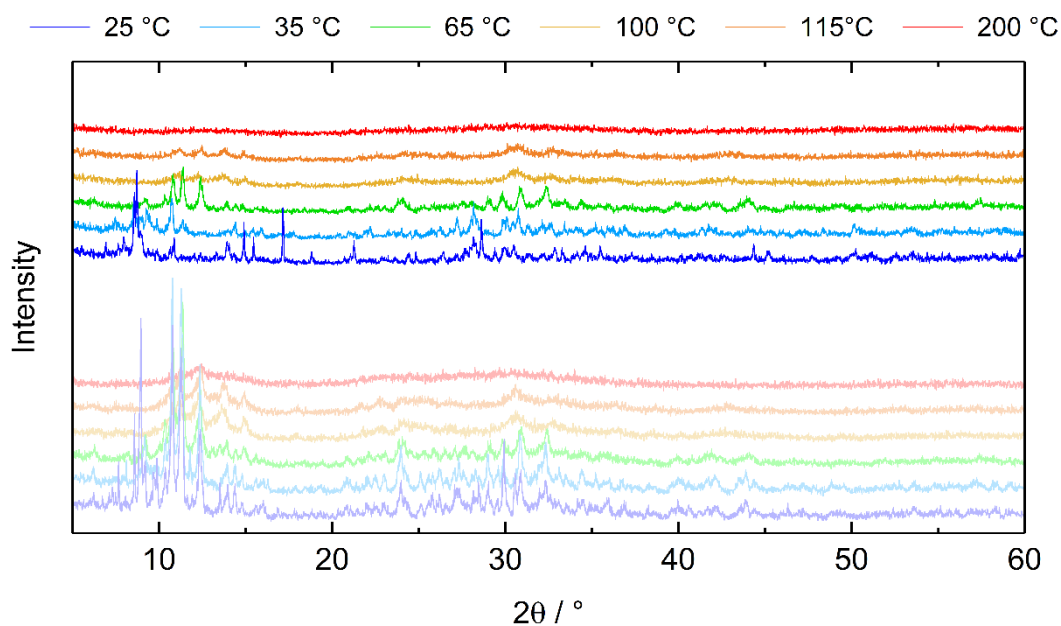
**Figure S3.** View of the asymmetric unit with hydrogen bonds network represented in dashes. Light blue and red dashes correspond to intra- and inter-molecular H bonds respectively.



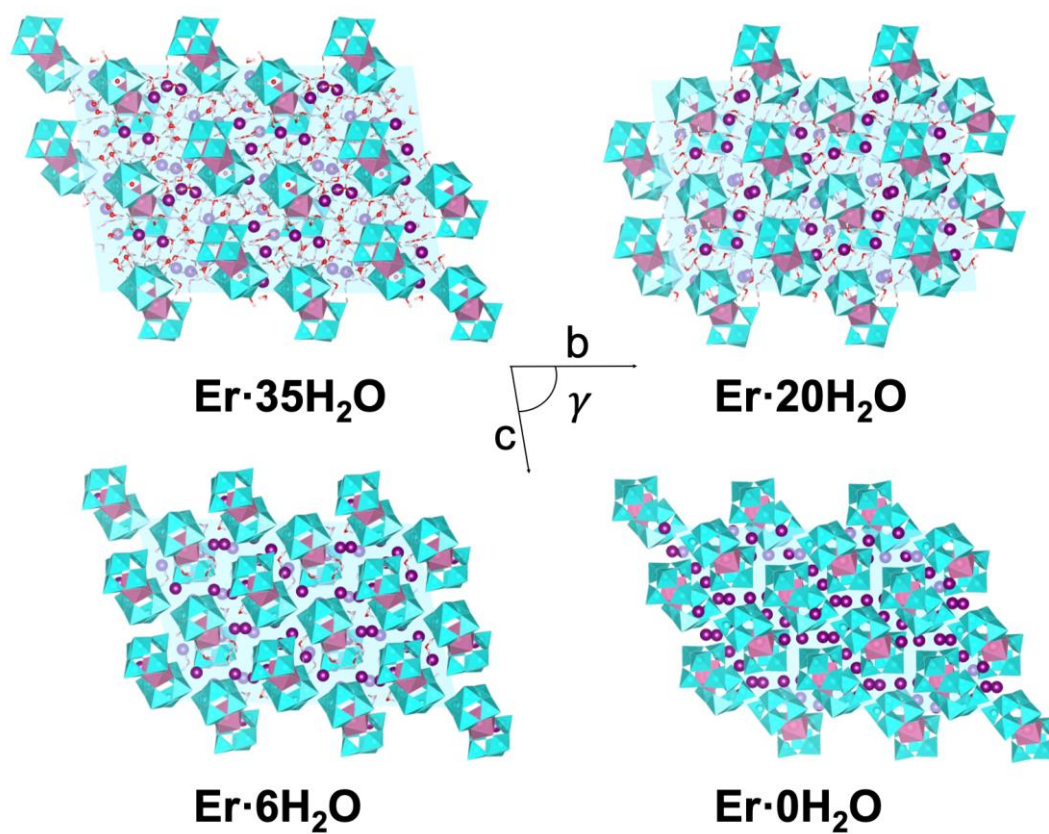
**Figure S4.** Three different TGA/TDA cycles of  $\text{Er}\cdot 35\text{H}_2\text{O}$ . The initial sample is represented in black, the red curve corresponds to the rehydrated sample and in pink after the second rehydration process. The grey dashed lines separate the different weight losses.



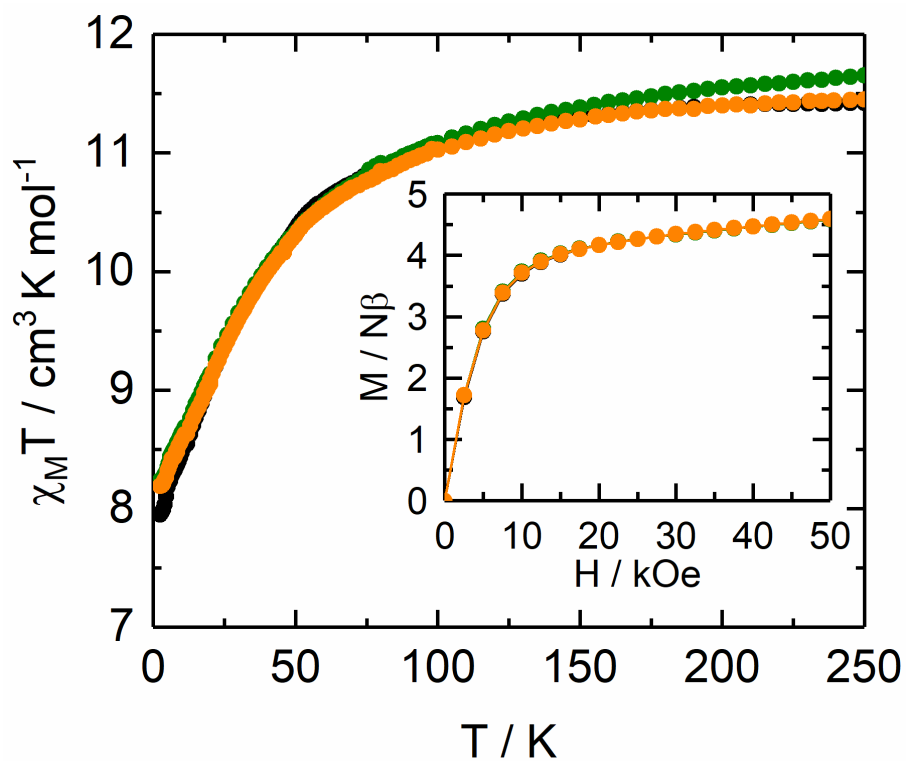
**Figure S5.** Experimental room temperature powder X-ray diffractogram of **Er·35H<sub>2</sub>O** with the simulated one from single crystal X-ray diffraction structure obtained at -123°C.



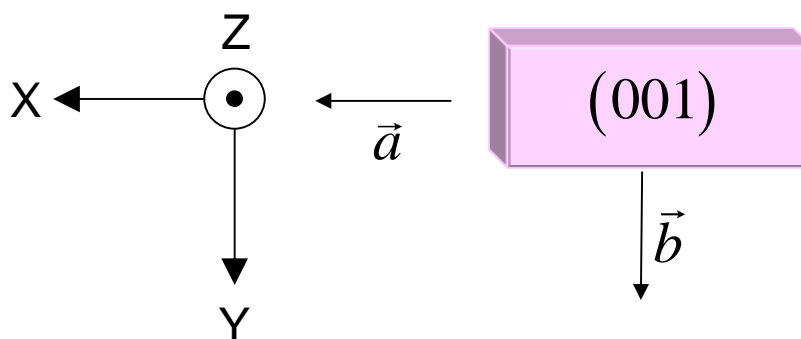
**Figure S6.** Selected diffractograms from the Temperature Dependant X-ray Powder Diffraction (TDXD) measurements of **Er·35H<sub>2</sub>O** from 25 to 200°C. Light colours correspond to the first heat of the sample starting from the crystalline state and bright colours to the second heat after room temperature rehydration procedure in air.



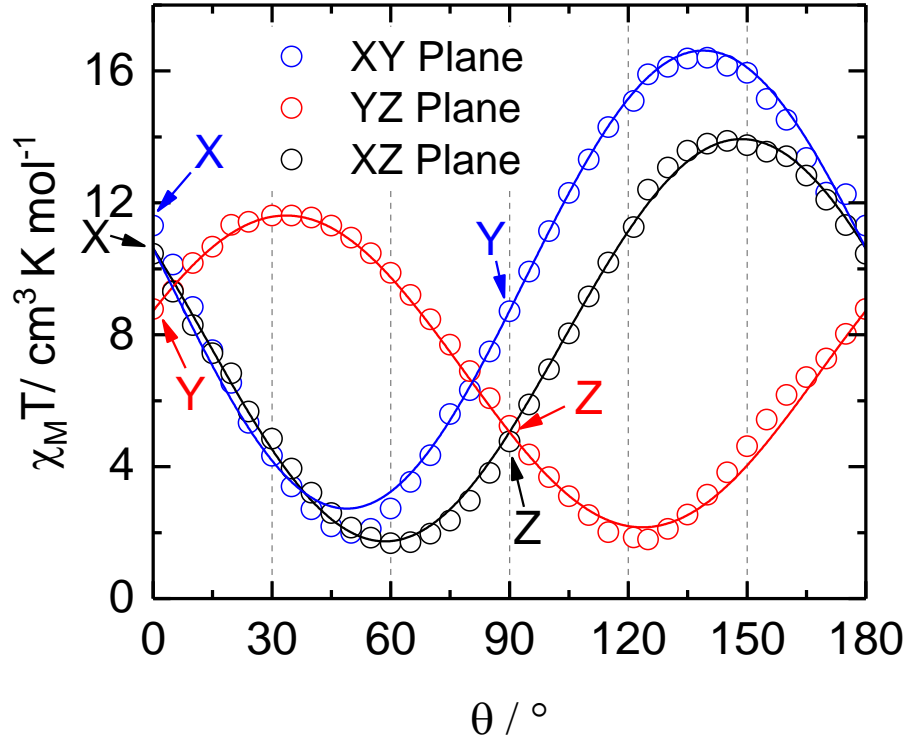
**Figure S7.** Evolution of the crystal packing upon dehydration. The crystal packing is plotted in the *bc* plane for each optimized structure. The O, Na and H atoms are represented as red, white and purple spheres while the Er<sup>III</sup> and (W<sub>5</sub>O<sub>18</sub>)<sup>6-</sup> ions are represented as pink and cyan polygons.



**Figure S8.** Thermal dependence of the  $\chi_M T$  for  $^{167}\text{Er}\cdot 35\text{H}_2\text{O}$  (olive),  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  (orange) and  $\text{Er}\cdot 35\text{H}_2\text{O}$  (black). The inset shows the field variation of the magnetization at 2 K (lines are guides for eyes only).



**Figure S9.** Oriented single crystal of  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  with the XYZ crystal reference frame.



**Figure S10.** Angular dependence of  $\chi_M T$  of a single crystal rotating in three perpendicular planes with  $H = 1$  kOe at 2 K for  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$ . Full lines are best-fitted curves (see text).

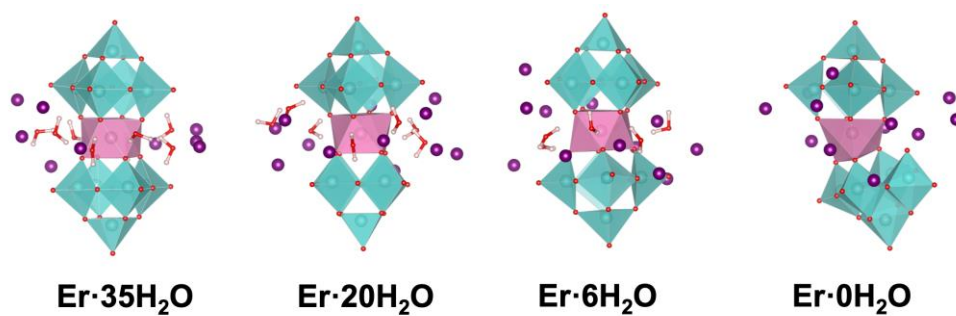
Susceptibility tensor in the crystal frame (XYZ):

$$\chi_M T = \begin{pmatrix} 10.620 & -6.88 & -5.427 \\ -6.88 & 8.728 & 4.355 \\ -5.427 & 4.355 & 5.05 \end{pmatrix} \text{cm}^3 \text{K mol}^{-1}$$

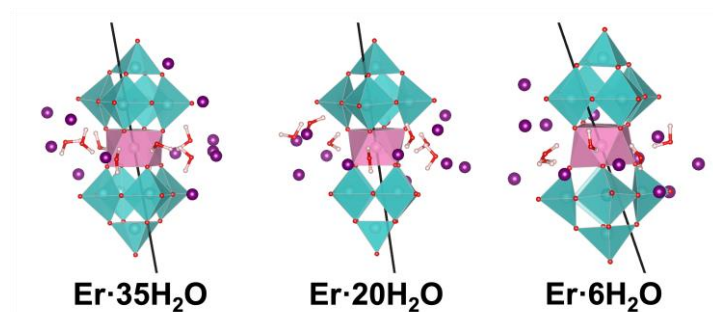
Principal values and direction of the susceptibility tensor in the XYZ crystal frame:

$$\chi_{xx} T \begin{pmatrix} -0.472 \\ 0.082 \\ -0.878 \end{pmatrix} = 1.724, \quad \chi_{yy} T \begin{pmatrix} -0.553 \\ -0.803 \\ 0.222 \end{pmatrix} = 2.793, \quad \chi_{zz} T \begin{pmatrix} -0.687 \\ 0.590 \\ 0.425 \end{pmatrix} = 19.88 \text{ cm}^3 \text{K mol}^{-1}$$

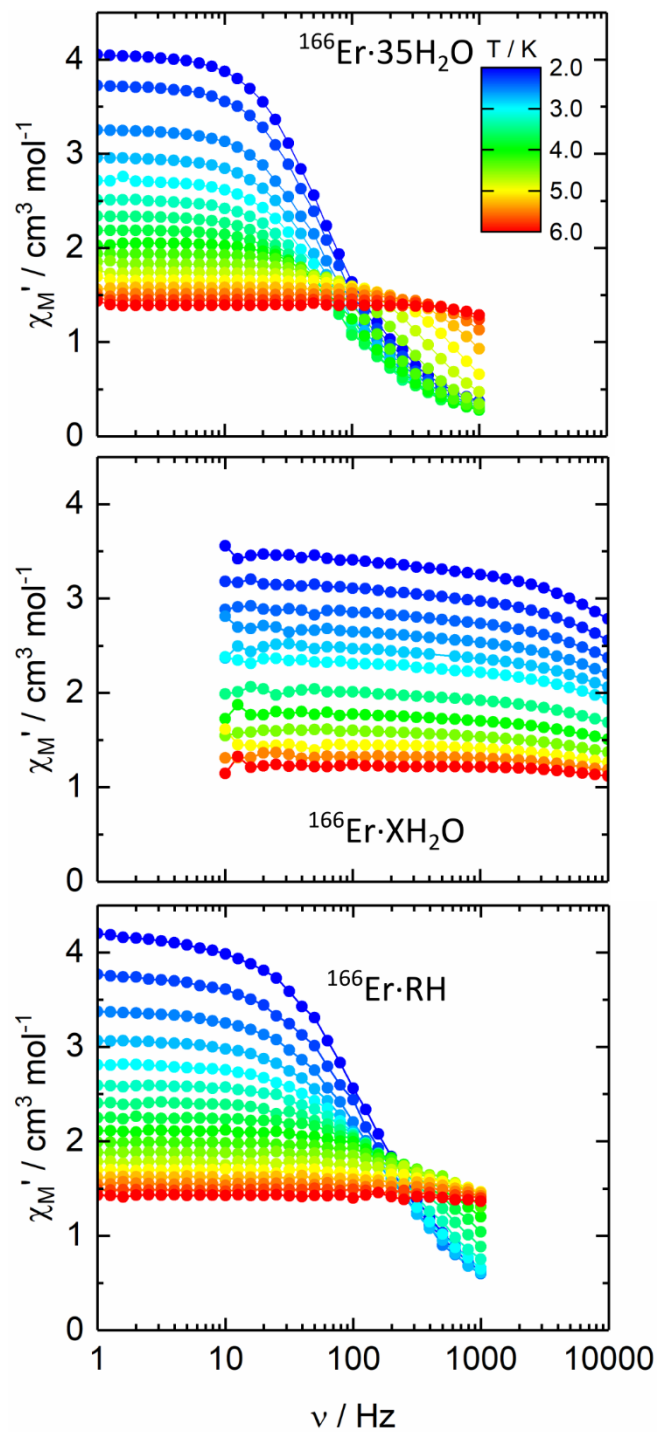




**Figure S11.** Models used for the CASSCF calculations. The O, Na and H atoms are represented as red, white and purple spheres while the Er<sup>III</sup> and (W<sub>5</sub>O<sub>18</sub>)<sup>6-</sup> ions are represented as pink and cyan polygons.



**Figure S12.** Evolution of the computed main component of the ground state anisotropy axis ( $g_{zz}$ ).



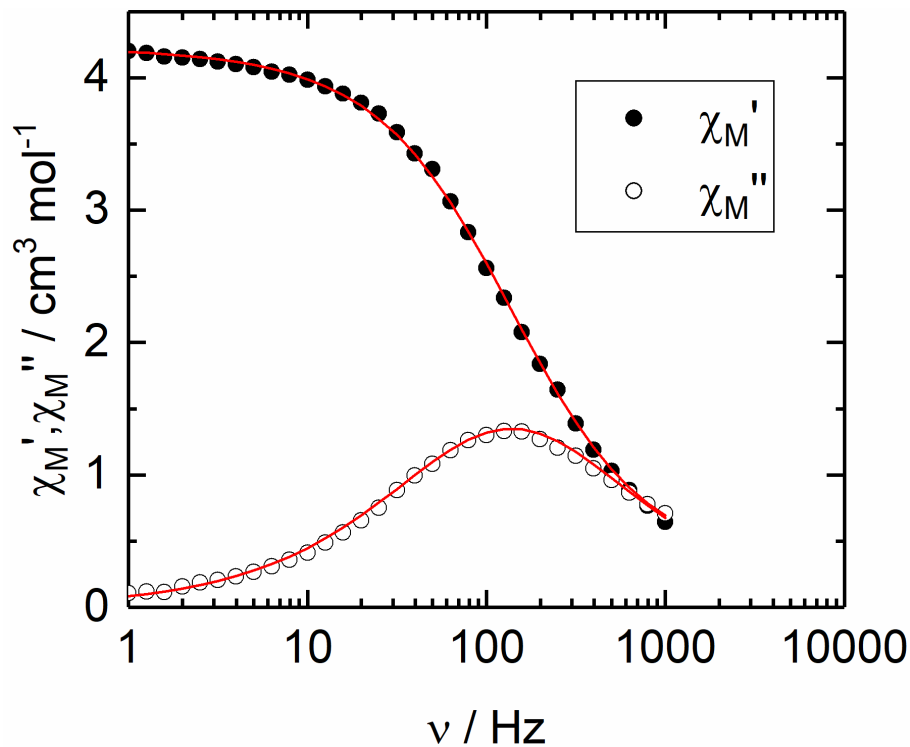
**Figure S13.** Frequency dependencies of the in-phase component,  $\chi_M'$ , of the ac susceptibility for three different solvation states of the isotopically enriched  $^{166}\text{Er}$  derivative, measured in zero external dc field and at various temperatures.

### Extended Debye model.

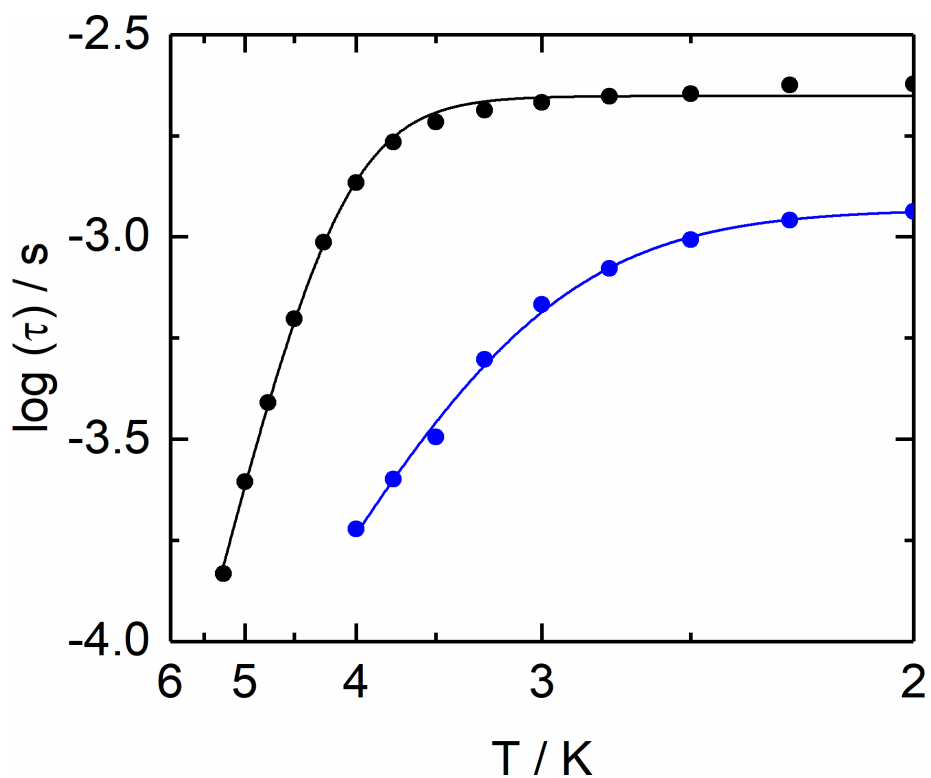
$$\chi_M' = \chi_S + (\chi_T - \chi_S) \frac{1 + (\omega\tau)^{1-\alpha} \sin\left(\alpha \frac{\pi}{2}\right)}{1 + 2(\omega\tau)^{1-\alpha} \sin\left(\alpha \frac{\pi}{2}\right) + (\omega\tau)^{2-2\alpha}}$$

$$\chi_M'' = (\chi_T - \chi_S) \frac{(\omega\tau)^{1-\alpha} \cos\left(\alpha \frac{\pi}{2}\right)}{1 + 2(\omega\tau)^{1-\alpha} \sin\left(\alpha \frac{\pi}{2}\right) + (\omega\tau)^{2-2\alpha}}$$

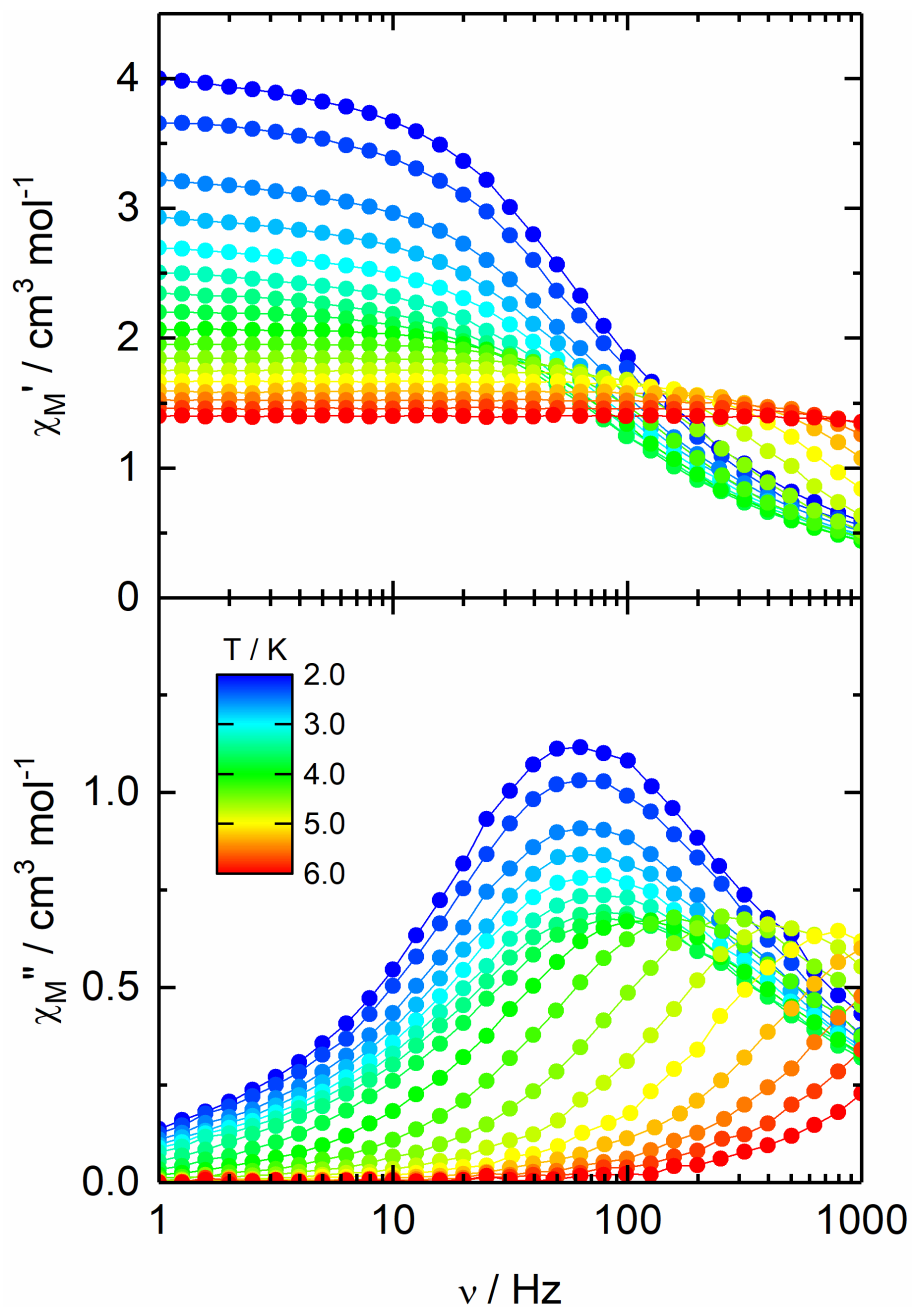
With  $\chi_T$  the isothermal susceptibility,  $\chi_S$  the adiabatic susceptibility,  $\tau$  the relaxation time and  $\alpha$  an empiric parameter which describe the distribution of the relaxation time. For SMM with only one relaxing object  $\alpha$  is close to zero. The extended Debye model was applied to fit simultaneously the experimental variations of  $\chi_M'$  and  $\chi_M''$  with the frequency  $\nu$  of the oscillating field ( $\omega = 2\pi\nu$ ). Typically, only the temperatures for which a maximum on the  $\chi_M''$  vs.  $\nu$  curves, have been considered (see Figure S13 for an example). The best fitted parameters  $\tau$ ,  $\alpha$ ,  $\chi_T$ ,  $\chi_S$  are listed in tables hereunder with the coefficient of determination  $R^2$ .



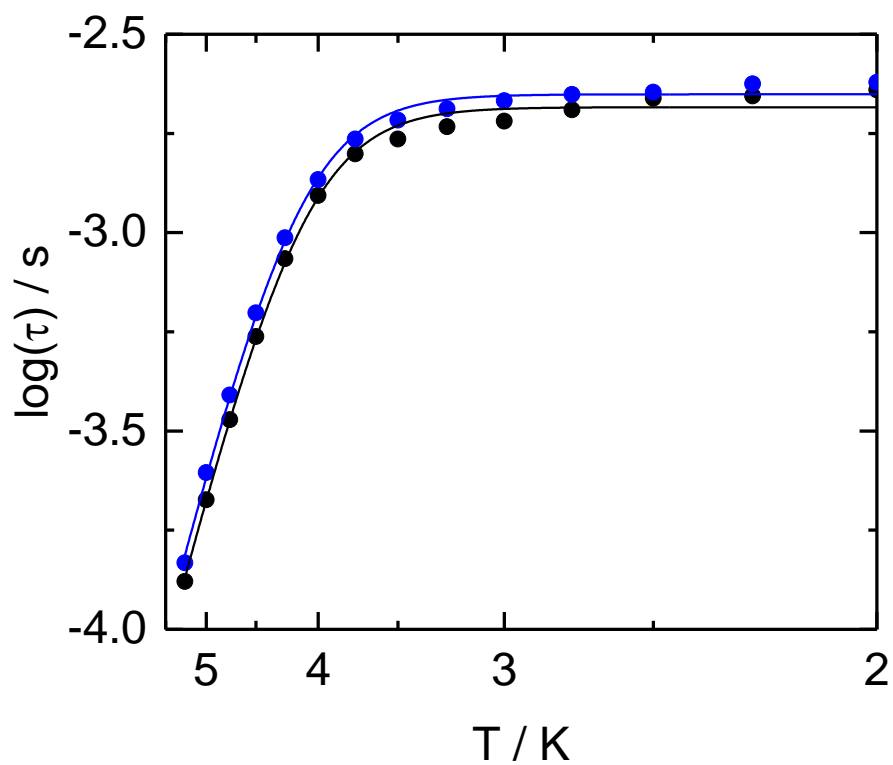
**Figure S14.** Frequency dependence of the in-phase (black dots) and out-of-phase (red dots) components of the ac susceptibility measured on powder at 2 K in zero external dc field with the best fitted curves (full lines) for  $^{166}\text{Er}\cdot\text{RH}$ .



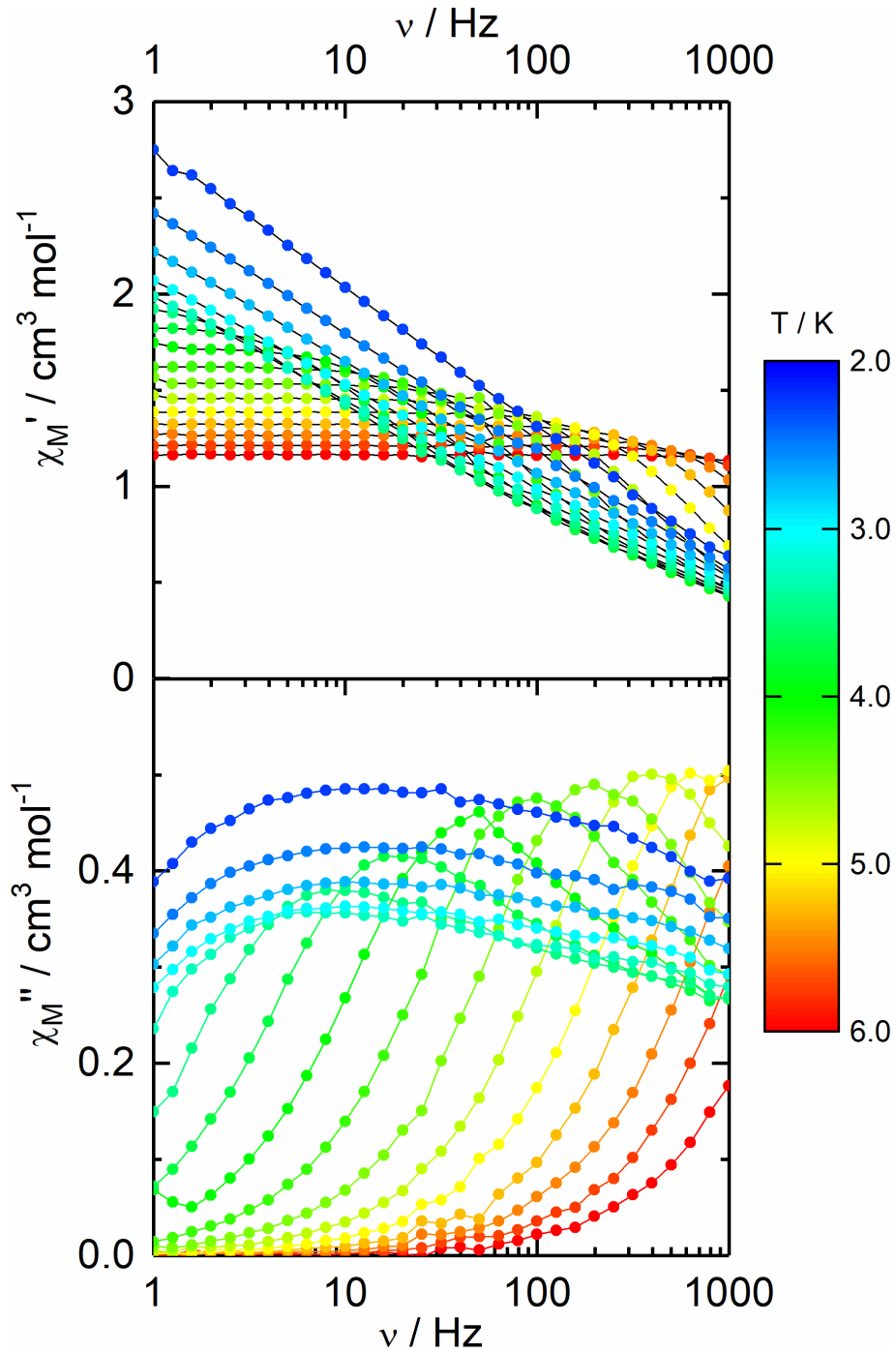
**Figure S15.** Temperature dependence of the relaxation times between 2 and 5.25 K at zero external dc field for  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  (black dots) and  $^{166}\text{Er}\cdot \text{RH}$  (blue dots). Full lines correspond to the best fitted curves with a combination of Orbach and thermally independent processes (see text).



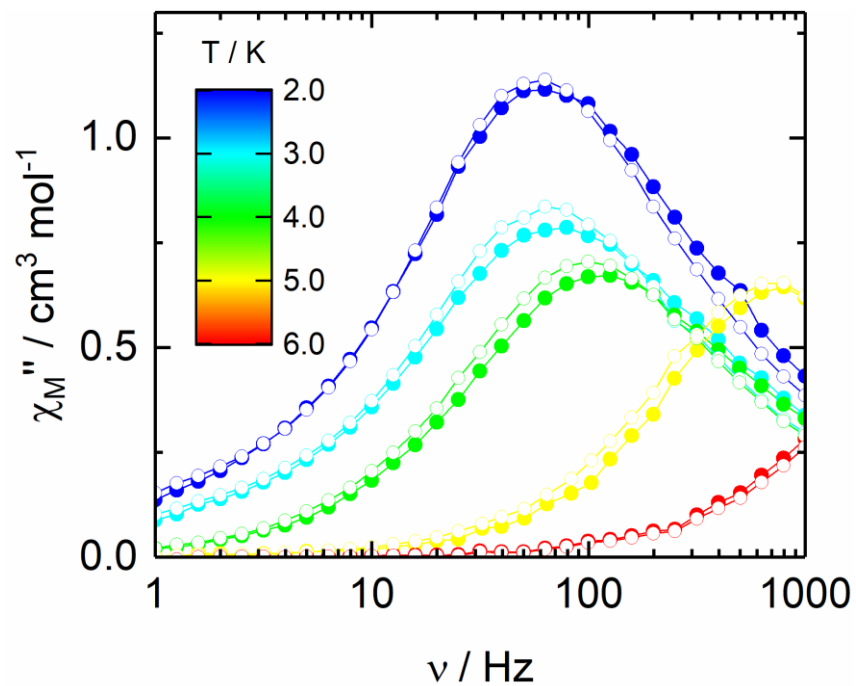
**Figure S16.** Frequency dependencies of the in-phase component (top),  $\chi_M'$ , and the out-of-phase component (bottom),  $\chi_M''$ , of the ac susceptibility for **Er·35H<sub>2</sub>O**, measured in zero external dc field and at various temperatures.



**Figure S17.** Temperature dependence of the relaxation times between 2 and 5.25 K at zero external dc field for  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  (blue dots) and  $\text{Er}\cdot 35\text{H}_2\text{O}$  (black dots). Full lines correspond to the best fitted curves.



**Figure S18.** Frequency dependencies of the in-phase component (top),  $\chi_M'$ , and the out-of-phase component (bottom),  $\chi_M''$ , of the ac susceptibility of a second batch of  $^{167}\text{Er}\cdot 35\text{H}_2\text{O}$ , measured in zero external dc field and at various temperatures.



**Figure S19.** Frequency dependencies of the out-of-phase component,  $\chi_M''$ , of the ac susceptibility for  $\text{Er}\cdot 35\text{H}_2\text{O}$  (full dots) and weighted sum (77%  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  + 23%  $^{167}\text{Er}\cdot 35\text{H}_2\text{O}$ ) measured in zero external dc field and at various temperatures.



**Table S1.** Mass number, abundance and nuclear spin values of the stable lanthanide isotopes.

Lanthanide	Mass number	Abundance (%)	Nuclear spin
<b>La</b>	139	99.91	I=7/2
	138	0.09	I=5
<b>Ce</b>	136	0.185	I=0
	138	0.251	I=0
	140	88.45	I=0
	142	11.11	I=0
<b>Pr</b>	141	100	I=5/2
<b>Nd</b>	142	27.2	I=0
	143	12.2	I=7/2
	144	23.8	I=0
	145	8.3	I=7/2
	146	17.2	I=0
	148	5.7	I=0
	150	5.6	I=0
<b>Pm</b>	No stable isotope		
<b>Sm</b>	144	3.1%	I=0
	146	Traces	I=0
	147	14.99%	I=7/2
	148	11.24%	I=0
	149	13.82%	I=7/2
	150	7.38%	I=0
	152	26.75%	I=0
	154	22.75%	I=0
<b>Eu</b>	151	47.81%	I=5/2
	153	52.19%	I=5/2
<b>Gd</b>	152	0.2%	I=0
	154	2.18%	I=0
	155	14.8%	I=3/2
	156	20.47%	I=0
	157	15.65%	I=3/2
	158	24.84%	I=0
	160	21.86%	I=0
<b>Tb</b>	159	100%	I=3/2
<b>Dy</b>	156	0.056%	I=0
	158	0.095%	I=0
	160	2.329%	I=0
	161	18.889%	I=5/2
	162	25.475%	I=0
	163	24.896%	I=5/2
	164	28.26%	I=0
<b>Ho</b>	165	100%	I=7/2
<b>Er</b>	162	0.139%	I=0
	164	1.601%	I=0
	166	33.503%	I=0
	167	22.869%	I=7/2
	168	26.978%	I=0
	170	14.91%	I=0

<b>Tm</b>	169	100%	I=1/2
<b>Yb</b>	168	0.13%	I=0
	170	3.04%	I=0
	171	14.28%	I=1/2
	172	21.83%	I=0
	173	16.13%	I=5/2
	174	31.83%	I=0
	176	12.76%	I=0
<b>Lu</b>	175	97.41%	I=7/2
	176	2.59%	I=7

**Table S2.** Crystallographic data for **Er·35H<sub>2</sub>O**.

Compounds	Na <sub>9</sub> [Er(W <sub>5</sub> O <sub>18</sub> ) <sub>2</sub> ]·35H <sub>2</sub> O (Er·35H <sub>2</sub> O)
<b>Formula</b>	Na <sub>9</sub> ErW <sub>10</sub> O <sub>71</sub> H <sub>70</sub>
<b>M / g.mol<sup>-1</sup></b>	3418.67
<b>Crystal system</b>	Triclinic
<b>Space group</b>	P-1
<b>Cell parameters</b>	a = 12.7812(6) Å b = 13.0943(7) Å c = 20.5479(11) Å α = 82.822(2)° β = 74.707(2)° γ = 88.805(2)°
<b>Volume / Å<sup>3</sup></b>	3290.9(3)
<b>Cell formula units</b>	2
<b>T / K</b>	150(2)
<b>Diffraction reflection / °</b>	2.24 ≤ 2θ ≤ 27.55
<b>ρ<sub>calc</sub> / g cm<sup>-3</sup></b>	1.607
<b>μ / mm<sup>-1</sup></b>	18.843
<b>Number of reflections</b>	52171
<b>Independent reflections</b>	15021
<b>Fo<sup>2</sup> &gt; 2σ(Fo)<sup>2</sup></b>	12484
<b>Number of variables</b>	766
<b>R<sub>int</sub>, R<sub>1</sub>, wR<sub>2</sub></b>	0.0727, 0.0625, 0.1769

**Table S3.** Unit cell parameters for **<sup>166</sup>Er·35H<sub>2</sub>O** and **<sup>167</sup>Er·35H<sub>2</sub>O**.

Compounds	Na <sub>9</sub> [ <sup>166</sup> Er(W <sub>5</sub> O <sub>18</sub> ) <sub>2</sub> ]·35H <sub>2</sub> O ( <sup>166</sup> Er·35H <sub>2</sub> O)	Na <sub>9</sub> [ <sup>167</sup> Er(W <sub>5</sub> O <sub>18</sub> ) <sub>2</sub> ]·35H <sub>2</sub> O ( <sup>167</sup> Er·35H <sub>2</sub> O)
<b>Crystal system</b>	triclinic	triclinic
<b>Cell parameters</b>	a = 12.75(1) Å	a = 12.763(4) Å
	b = 13.07(1) Å	b = 13.117(5) Å
	c = 20.57(2) Å	c = 20.52(1) Å
	α = 82.89(2)°	α = 82.82(3)°
	β = 74.68(2)°	β = 74.41(2)°
	γ = 88.76(2)°	γ = 88.81(2)°
<b>Volume / Å<sup>3</sup></b>	3282(8)	3283(4)
<b>T / K</b>	293(2)	150(2)

**Table S4.** SHAPE analysis of the ErO<sub>8</sub> coordination polyhedron at various hydration stages.

The fully dehydrated material is not taken into account since Er<sup>III</sup> is heptacoordinated.

Compound	CShM <sub>SAPR-8</sub> square antiprism D <sub>4d</sub>	CShM <sub>TDD-8</sub> triangular dodecahedron D <sub>2d</sub>	CShM <sub>BTPR-8</sub> biaugmented trigonal prism C <sub>2v</sub>
Er·35H <sub>2</sub> O	0.046	2.647	<b>2.078</b>
Er·20H <sub>2</sub> O	0.453	1.973	<b>2.556</b>
Er·6H <sub>2</sub> O	1.412	2.177	<b>3.400</b>

**Table S5.** Computed energy levels (in cm<sup>-1</sup>; the ground state is set at zero) and composition of the *g*-tensor (*g*<sub>xx</sub>, *g*<sub>yy</sub> and *g*<sub>zz</sub> from top to bottom) of the <sup>4</sup>I<sub>15/2</sub> ground state multiplet of Er<sup>III</sup>.

KD	Er·35H <sub>2</sub> O		Er·20H <sub>2</sub> O		Er·6H <sub>2</sub> O		Er·0H <sub>2</sub> O	
	E	<i>g</i>	E	<i>g</i>	E	<i>g</i>	E	<i>g</i>
1	0	0.00	0	0.05	0	0.33	0	0.10
		0.01		0.11		0.71		1.45
		15.90		15.57		15.36		14.23
2	29	0.00	27	0.01	50	0.26	33	2.19
		0.00		0.01		0.27		3.60
		17.90		17.61		17.12		10.99
3	110	11.93	80	1.25	93	2.58	58	2.69
		6.87		6.30		6.17		4.16
		1.26		11.78		11.02		9.84
4	151	0.05	109	1.86	101	1.29	118	0.83
		0.35		3.28		2.02		2.59
		12.59		7.47		9.84		11.91
5	169	3.91	181	1.60	226	1.74	178	0.55
		3.09		2.63		2.40		2.76
		1.76		9.24		11.91		10.47
6	245	0.05	232	6.47	290	0.96	226	1.96
		1.43		4.14		3.50		3.95
		6.85		1.55		10.99		9.95
7	278	0.00	263	0.41	306	0.15	272	9.53
		0.76		1.30		1.99		5.27
		9.89		12.21		11.43		0.49
8	307	0.41	295	0.47	369	0.30	295	0.88
		1.51		0.63		0.49		4.35
		9.69		13.00		15.21		11.91

**Table S6.** Computed wavefunction for each  $M_J$  state of the ground-state multiplet of the  $\text{Er}^{\text{III}}$  centre. Only the contributions higher than 10% are mentioned.

KD	Er·35H <sub>2</sub> O	Er·20H <sub>2</sub> O	Er·6H <sub>2</sub> O	Er·0H <sub>2</sub> O
<b>1</b>	58% $ \pm 13/2\rangle +$ 29% $ \pm 15/2\rangle +$ 11% $ \pm 11/2\rangle$	51% $ \pm 13/2\rangle +$ 32% $ \pm 15/2\rangle +$ 13% $ \pm 11/2\rangle$	53% $ \pm 15/2\rangle +$ 20% $ \pm 13/2\rangle +$ 14% $ \pm 11/2\rangle$	44% $ \pm 11/2\rangle +$ 44% $ \pm 15/2\rangle$
<b>2</b>	70% $ \pm 15/2\rangle +$ 26% $ \pm 13/2\rangle$	65% $ \pm 15/2\rangle +$ 28% $ \pm 13/2\rangle$	40% $ \pm 15/2\rangle +$ 36% $ \pm 13/2\rangle +$ 12% $ \pm 11/2\rangle$	24% $ \pm 9/2\rangle +$ 24% $ \pm 7/2\rangle +$ 23% $ \pm 13/2\rangle$
<b>3</b>	52% $ \pm 1/2\rangle +$ 36% $ \pm 3/2\rangle$	59% $ \pm 1/2\rangle +$ 32% $ \pm 3/2\rangle$	33% $ \pm 3/2\rangle +$ 26% $ \pm 5/2\rangle +$ 20% $ \pm 1/2\rangle$	34% $ \pm 3/2\rangle +$ 17% $ \pm 5/2\rangle +$ 13% $ \pm 9/2\rangle$
<b>4</b>	64% $ \pm 11/2\rangle +$ 15% $ \pm 13/2\rangle +$ 13% $ \pm 9/2\rangle$	24% $ \pm 11/2\rangle +$ 22% $ \pm 3/2\rangle +$ 22% $ \pm 5/2\rangle$	29% $ \pm 1/2\rangle +$ 17% $ \pm 7/2\rangle +$ 13% $ \pm 5/2\rangle$	31% $ \pm 13/2\rangle +$ 15% $ \pm 15/2\rangle +$ 13% $ \pm 7/2\rangle$
<b>5</b>	42% $ \pm 1/2\rangle +$ 27% $ \pm 5/2\rangle$	34% $ \pm 11/2\rangle +$ 16% $ \pm 1/2\rangle +$ 16% $ \pm 5/2\rangle$	26% $ \pm 11/2\rangle +$ 21% $ \pm 13/2\rangle +$ 14% $ \pm 7/2\rangle$	24% $ \pm 1/2\rangle +$ 18% $ \pm 9/2\rangle +$ 16% $ \pm 7/2\rangle$
<b>6</b>	32% $ \pm 3/2\rangle +$ 24% $ \pm 9/2\rangle +$ 20% $ \pm 5/2\rangle$	45% $ \pm 7/2\rangle +$ 27% $ \pm 3/2\rangle +$ 14% $ \pm 5/2\rangle$	43% $ \pm 9/2\rangle +$ 18% $ \pm 7/2\rangle +$ 17% $ \pm 1/2\rangle$	24% $ \pm 1/2\rangle +$ 19% $ \pm 13/2\rangle +$ 18% $ \pm 7/2\rangle$
<b>7</b>	44% $ \pm 9/2\rangle +$ 32% $ \pm 7/2\rangle +$ 15% $ \pm 11/2\rangle$	72% $ \pm 9/2\rangle +$ 21% $ \pm 11/2\rangle$	31% $ \pm 11/2\rangle +$ 27% $ \pm 7/2\rangle +$ 15% $ \pm 3/2\rangle$	26% $ \pm 5/2\rangle +$ 23% $ \pm 11/2\rangle +$ 18% $ \pm 7/2\rangle$
<b>8</b>	42% $ \pm 7/2\rangle +$ 40% $ \pm 5/2\rangle +$ 13% $ \pm 9/2\rangle$	42% $ \pm 7/2\rangle +$ 40% $ \pm 5/2\rangle +$ 12% $ \pm 3/2\rangle$	37% $ \pm 5/2\rangle +$ 25% $ \pm 3/2\rangle +$ 15% $ \pm 7/2\rangle$	26% $ \pm 3/2\rangle +$ 19% $ \pm 11/2\rangle +$ 18% $ \pm 1/2\rangle$

**Table S7.** Best fitted parameters ( $\chi_T$ ,  $\chi_S$ ,  $\tau$  and  $\alpha$ ) with the extended Debye model for compound  $^{166}\text{Er}\cdot 35\text{H}_2\text{O}$  in zero external dc field between 2 and 5.25 K.

T / K	$\chi_S / \text{cm}^3 \text{mol}^{-1}$	$\chi_T / \text{cm}^3 \text{mol}^{-1}$	$\tau / \text{s}$	$\alpha$	R <sup>2</sup>
<b>2</b>	0.33604	4.08724	0.00239	0.13737	0.9987
<b>2.25</b>	0.32312	3.76075	0.00237	0.13525	0.99926
<b>2.5</b>	0.27966	3.2915	0.00226	0.14416	0.99931
<b>2.75</b>	0.26295	2.99323	0.00223	0.14202	0.99923
<b>3</b>	0.25474	2.7475	0.00215	0.13944	0.99752
<b>3.25</b>	0.23138	2.54497	0.00205	0.14756	0.99934
<b>3.5</b>	0.21404	2.36851	0.00192	0.14289	0.99936
<b>3.75</b>	0.21266	2.21432	0.00172	0.12757	0.99919
<b>4</b>	0.21174	2.06672	0.00136	0.10393	0.99903
<b>4.25</b>	0.19048	1.95223	9.70294E-4	0.08844	0.99966
<b>4.5</b>	0.17831	1.83714	6.27211E-4	0.07376	0.99204
<b>4.75</b>	0.1583	1.74471	3.89598E-4	0.06635	0.99996
<b>5</b>	0.17142	1.65865	2.48379E-4	0.05963	0.99996
<b>5.25</b>	0.15849	1.57712	1.47087E-4	0.06439	0.99949

**Table S8.** Best fitted parameters ( $\chi_T$ ,  $\chi_S$ ,  $\tau$  and  $\alpha$ ) with the extended Debye model for compound  $^{166}\text{Er}\cdot\text{RH}$  in zero external dc field between 2 and 4 K.

T / K	$\chi_S / \text{cm}^3 \text{mol}^{-1}$	$\chi_T / \text{cm}^3 \text{mol}^{-1}$	$\tau / \text{s}$	$\alpha$	$R^2$
2	0.26678	4.23164	0.00116	0.23874	0.99982
2.25	0.22256	3.83946	0.0011	0.2483	0.99964
2.5	0.21847	3.401	9.83963E-4	0.22871	0.99986
2.75	0.18363	3.08935	8.33973E-4	0.23285	0.99977
3	0.21017	2.83848	6.81564E-4	0.23222	0.99981
3.25	0.19122	2.62057	4.97027E-4	0.23762	0.9997
3.5	0.12296	2.43226	3.19775E-4	0.26397	0.99978
3.75	0.28004	2.26946	2.51636E-4	0.24702	0.99979
4	0.39657	2.12636	1.89629E-4	0.23781	0.99979

**Table S9.** Best fitted parameters ( $\chi_T$ ,  $\chi_S$ ,  $\tau$  and  $\alpha$ ) with the extended Debye model for compound  $\text{Er}\cdot 35\text{H}_2\text{O}$  in zero external dc field between 2 and 5.25 K.

T / K	$\chi_S / \text{cm}^3 \text{mol}^{-1}$	$\chi_T / \text{cm}^3 \text{mol}^{-1}$	$\tau / \text{s}$	$\alpha$	$R^2$
2	0.46215	4.04432	0.00229	0.24466	0.99923
2.25	0.42093	3.72717	0.00221	0.25014	0.99939
2.5	0.38057	3.26278	0.00218	0.25189	0.99954
2.75	0.32907	2.98122	0.00204	0.26078	0.99959
3	0.31035	2.73646	0.00191	0.26091	0.99979
3.25	0.29152	2.53693	0.00185	0.26051	0.9998
3.5	0.28803	2.371	0.00172	0.25332	0.99977
3.75	0.30929	2.22142	0.00158	0.21685	0.99954
4	0.32421	2.08371	0.00124	0.16284	0.99959
4.25	0.31927	1.96391	8.59423E-4	0.12159	0.99964
4.5	0.30394	1.85165	5.4717E-4	0.08515	0.9998
4.75	0.30703	1.75526	3.37699E-4	0.05543	0.9999
5	0.32615	1.66894	2.11899E-4	0.0291	0.99997
5.25	0.32972	1.59136	1.31963E-4	0.01531	0.99994

## xyz coordinates of models used for the CASSCF calculations

### Er·35H<sub>2</sub>O

Er	18.588432	11.368752	14.159699
W	19.162033	7.602680	14.251816
W	22.005146	10.844709	12.564884
W	18.237490	14.777709	15.829756
W	21.614206	9.437205	15.422224
W	22.178413	7.506615	12.743605
W	14.913759	15.115881	15.507310
W	19.523544	9.012556	11.271720
W	14.876415	12.074079	14.034856
W	16.856266	14.435333	12.860145
W	16.290310	12.402713	16.999744
O	17.581831	13.800027	17.401604
O	18.084267	15.460892	13.988613
O	22.706268	7.932961	14.565382
O	13.818641	13.696716	14.715774
O	19.238796	13.370317	15.272560
O	21.032307	7.646247	11.202257
O	16.516993	15.887188	16.127169
O	20.717026	6.515298	13.558627
O	14.975284	13.956754	17.075344
O	20.298616	10.670176	15.565636
O	22.705257	10.615925	14.341112
O	19.376688	15.865485	16.564501
O	15.395647	15.660728	13.726710
O	17.550856	11.321687	16.268467
O	20.965391	10.298280	10.953097
O	18.624640	7.621698	12.354975
O	18.029505	13.069985	12.671141
O	13.517238	11.183741	13.366523
O	16.429157	13.531025	14.950997
O	14.873637	11.537759	15.928093
O	18.508327	10.295948	12.040742
O	20.631968	11.898062	13.106683
O	18.182243	9.088014	14.591050
O	15.322332	13.265600	12.567165
O	20.321846	7.971337	15.785032
O	16.306387	11.016539	13.686302
O	13.621364	16.267235	15.940548
O	15.987603	11.711490	18.585829
O	18.772707	8.735032	9.718377
O	18.168091	6.277105	14.855434
O	22.463383	9.517570	16.953465
O	16.931252	15.322824	11.359853
O	20.694693	9.096628	13.356022
O	23.033342	9.099222	12.164595
O	23.150942	11.943972	11.831527

O	23.329584	6.213541	12.362932
O	20.859842	12.040423	17.785763
O	15.773611	8.712785	15.760218
O	21.884123	14.510258	15.414878
O	15.937519	8.683329	12.275986
O	18.765797	9.372053	17.705282
O	20.632130	14.446453	12.394028
O	19.368050	12.547187	10.367772
O	16.610973	11.545115	10.050130
H	16.102388	9.575421	12.687436
H	16.840302	8.295412	12.209421
H	16.136662	10.722862	9.778932
H	17.262671	11.262212	10.728732
H	15.350850	9.596966	15.808663
H	16.701029	8.911258	15.464380
H	18.298346	10.053087	17.151463
H	19.302719	8.873366	17.048906
H	20.427692	11.799608	16.932371
H	20.437298	12.874810	18.126705
H	18.905693	12.735368	11.223487
H	19.969761	11.792486	10.553168
H	22.656006	14.009974	15.786348
H	21.108810	13.907741	15.397713
H	20.576622	13.480905	12.644918
H	19.866814	14.862132	12.835979
Na	14.865055	7.555436	13.987086
Na	21.492107	16.698257	16.174664
Na	22.438450	15.471045	13.344957
Na	17.037239	7.670067	8.586285
Na	14.380555	8.031881	10.618540
Na	12.297400	11.671291	9.760908
Na	19.536011	16.959391	9.443917
Na	17.658350	7.916643	19.037989
Na	23.148186	11.697738	17.601454
Na	12.341559	14.994914	10.771000
Na	19.491850	13.635767	8.433824
Na	14.898823	7.264612	17.377504

### **Er·20H<sub>2</sub>O**

Er	7.198766	10.807168	12.684236
W	7.912560	7.052971	13.018016
W	10.280464	10.235522	10.567035
W	7.017928	14.132296	14.620116
W	10.430135	9.105658	13.592268
W	10.601678	6.884534	11.061165
W	3.675972	14.537986	14.613155
W	7.801295	8.211108	9.892924
W	3.538037	11.626391	12.937361
W	5.355436	14.073715	11.778277

W 5.110296 11.774639 15.821157  
O 6.515945 13.091866 16.181135  
O 6.695529 14.940085 12.850105  
O 11.412060 7.559064 12.721185  
O 2.486685 13.232840 13.826327  
O 7.884766 12.763075 13.802667  
O 9.274995 6.853388 9.713544  
O 5.405833 15.251337 15.111811  
O 9.376773 5.923776 12.224466  
O 11.346744 8.462443 10.212114  
O 3.870983 13.345871 16.098423  
O 9.068734 10.263288 13.908097  
O 11.246436 10.218216 12.240841  
O 8.313695 15.121180 15.297364  
O 4.033627 15.163921 12.822912  
O 6.284389 10.751668 14.881988  
O 9.116971 9.485013 9.210242  
O 7.132378 6.897830 11.202585  
O 6.467676 12.658145 11.368112  
O 2.124123 10.786762 12.331560  
O 5.110395 12.998266 13.821183  
O 3.592079 10.999472 14.829195  
O 6.886115 9.570155 10.698460  
O 9.022226 11.320167 11.236568  
O 6.878833 8.526901 13.292265  
O 3.794504 12.878811 11.500067  
O 9.260669 7.640243 14.273545  
O 4.891546 10.547585 12.438448  
O 11.692475 5.563152 10.687384  
O 2.624403 15.868648 15.156752  
O 4.990026 10.970636 17.377031  
O 6.836392 7.839014 8.495581  
O 11.314143 11.276878 9.548549  
O 7.064530 5.784013 13.899764  
O 11.528503 9.365411 14.945049  
O 5.252009 14.971477 10.281075  
O 9.217972 8.550426 11.729942  
O 4.64578 7.86189 11.39092  
O 4.25570 8.42765 14.35660  
O 7.49306 8.75645 16.11980  
O 9.38603 10.96798 16.76204  
O 10.49524 12.79344 14.35821  
O 9.45694 15.18056 12.21595  
O 8.02230 13.46248 9.25230  
O 5.44085 11.22892 9.29865  
Na 3.029523 7.132915 12.858644  
Na 10.706107 14.814253 15.482970  
Na 11.704869 15.201057 11.488236  
Na 3.302378 6.926439 9.861290  
Na 1.196357 9.063828 8.536560



Na	8.039662	15.454461	7.948453
Na	9.179693	8.821109	17.706921
Na	6.216928	6.909095	16.388498
Na	11.522654	11.452481	16.094137
Na	1.751403	12.716106	9.870893
Na	6.802221	12.239128	7.711651
Na	3.111294	7.050935	15.799228
H	4.792471	8.810360	11.607538
H	5.554681	7.472622	11.378605
H	4.059340	9.372828	14.563552
H	5.151474	8.460765	13.939732
H	7.027056	9.512223	15.665369
H	8.134149	8.439194	15.439402
H	8.905506	10.933578	15.907487
H	8.974039	11.685161	17.308243
H	7.538126	13.167944	10.068809
H	8.970487	13.512580	9.544518
H	5.605199	11.849257	10.056549
H	5.911031	10.425761	9.668708
H	11.016310	12.923250	13.528674
H	9.577544	12.569016	14.067022
H	9.063719	15.797012	12.868554
H	8.981004	14.337944	12.357245

### **Er·6H<sub>2</sub>O**

W	18.119024	7.790617	11.903331
W	20.504440	10.797144	9.452093
W	16.470594	14.583714	13.025822
W	20.417004	10.041638	12.684837
W	21.088627	7.653434	10.427138
W	13.168604	14.863335	12.395128
W	18.258518	8.512035	8.757347
W	13.482270	12.005638	10.665506
W	15.393340	14.517740	9.917708
W	14.400424	12.095084	13.798560
Er	17.150965	11.351260	11.097318
O	15.702776	13.436506	14.424972
O	16.470596	15.383702	11.238864
O	21.562056	8.510804	12.079045
O	12.197255	13.534881	11.336654
O	17.492165	13.232485	12.380929
O	19.870302	7.294790	8.937036
O	14.707747	15.559791	13.270338
O	19.721043	6.681376	11.466944
O	21.752354	9.153561	9.460183
O	13.033562	13.565385	13.837492
O	18.913630	11.080073	12.696809
O	21.243567	11.072297	11.275038
O	17.692209	15.472947	13.913574

O	13.842784	15.577591	10.718192
O	15.829381	11.124344	13.183327
O	19.590988	9.803662	8.075315
O	17.493160	7.331685	10.095510
O	16.579100	13.158438	9.683511
O	12.311192	11.118240	9.710120
O	14.779268	13.370656	11.831642
O	13.195080	11.272099	12.478976
O	17.192705	9.929425	9.181357
O	19.082735	11.851093	9.881609
O	16.984779	9.225307	11.822670
O	13.965543	13.299602	9.283305
O	19.263302	8.537180	13.321281
O	14.960406	10.973083	10.433279
O	22.316240	6.406572	10.339406
O	11.941541	16.049984	12.845785
O	14.005590	11.354889	15.328316
O	17.409313	7.850461	7.376991
O	21.454119	11.808750	8.369123
O	17.168373	6.783252	12.962352
O	21.354198	10.721065	14.019044
O	15.728500	15.503904	8.483519
O	19.436039	9.195073	10.684052
O	19.609436	13.287851	14.291919
O	14.495099	8.382029	12.425027
O	14.601947	8.685262	9.050369
O	16.826633	9.114860	14.625301
O	19.539299	14.452528	10.241677
O	17.405073	11.341058	6.877100
H	14.860877	9.524479	9.541683
H	15.266595	8.635249	8.337048
H	13.769864	9.033678	12.489678
H	15.314425	8.931666	12.262358
H	16.252174	9.737787	14.099908
H	17.678541	9.162517	14.130238
H	19.291407	12.838451	13.465248
H	19.003891	14.062050	14.404265
H	18.164064	11.914156	7.113133
H	17.284128	10.767771	7.681683
H	19.306303	13.493908	10.066911
H	19.139423	14.632643	11.114116
Na	15.114270	7.011813	10.590651
Na	21.860409	14.976891	10.470637
Na	17.906090	10.768378	4.709325
Na	12.362996	9.064054	8.680145
Na	18.413277	15.860189	8.826905
Na	17.643982	11.708597	14.788015
Na	18.367544	7.405068	15.571909
Na	22.677719	12.230561	12.916509
Na	12.141268	12.648772	7.873725

Na	16.088505	13.096497	7.306237
Na	20.702881	11.985881	16.048241
Na	15.308646	7.127783	14.311684