**Supporting Information**

for paper

# Synthesis, structural features, magnetic properties and thermal decomposition of a new series of polymeric Ln(III)-Cr(III) cyclopropane-1,1-dicarboxylates

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## I. X-ray powder diffraction patterns

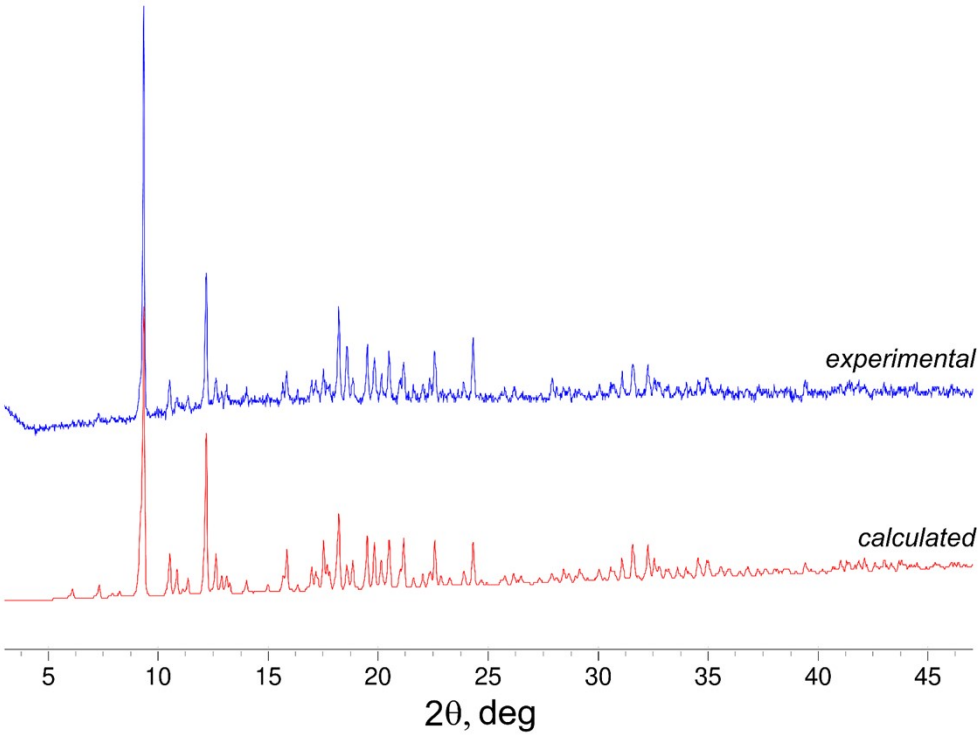



**Fig. S1.** The experimental PXRD pattern for $\mathbf{1}_{\mathbf{Eu}}$ measured at 295 K and its comparison with calculated data for $\mathbf{1}_{\mathbf{Eu}}$.

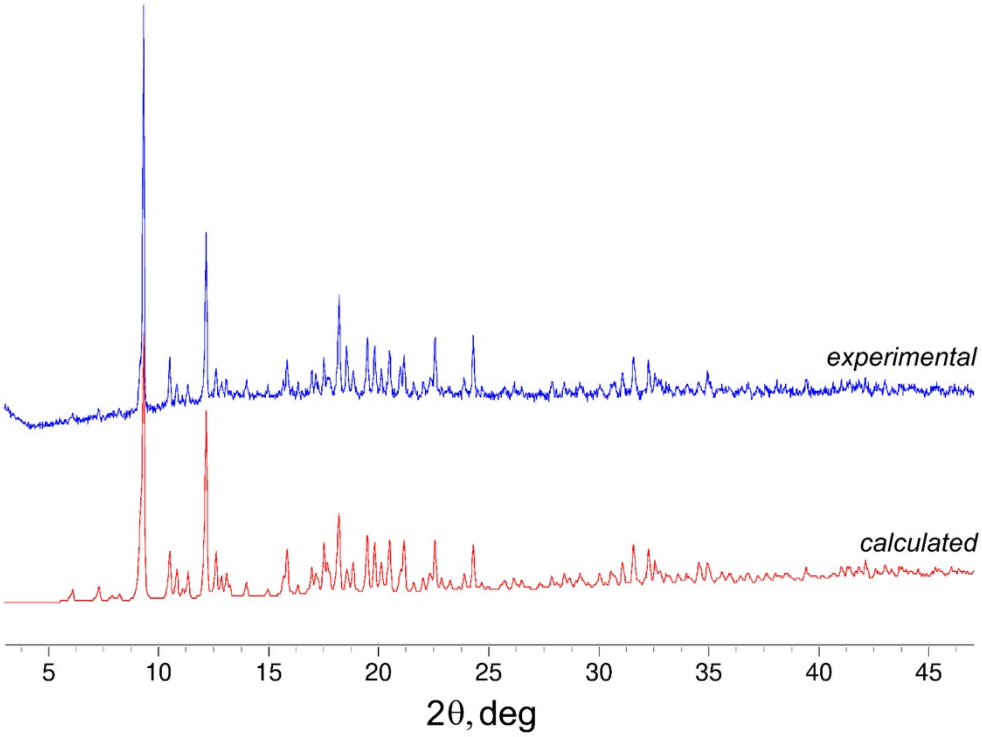



**Fig. S2.** The experimental PXRD pattern for $\mathbf{1}_{\mathbf{Gd}}$ measured at 295 K and its comparison with calculated data for $\mathbf{1}_{\mathbf{Gd}}$.

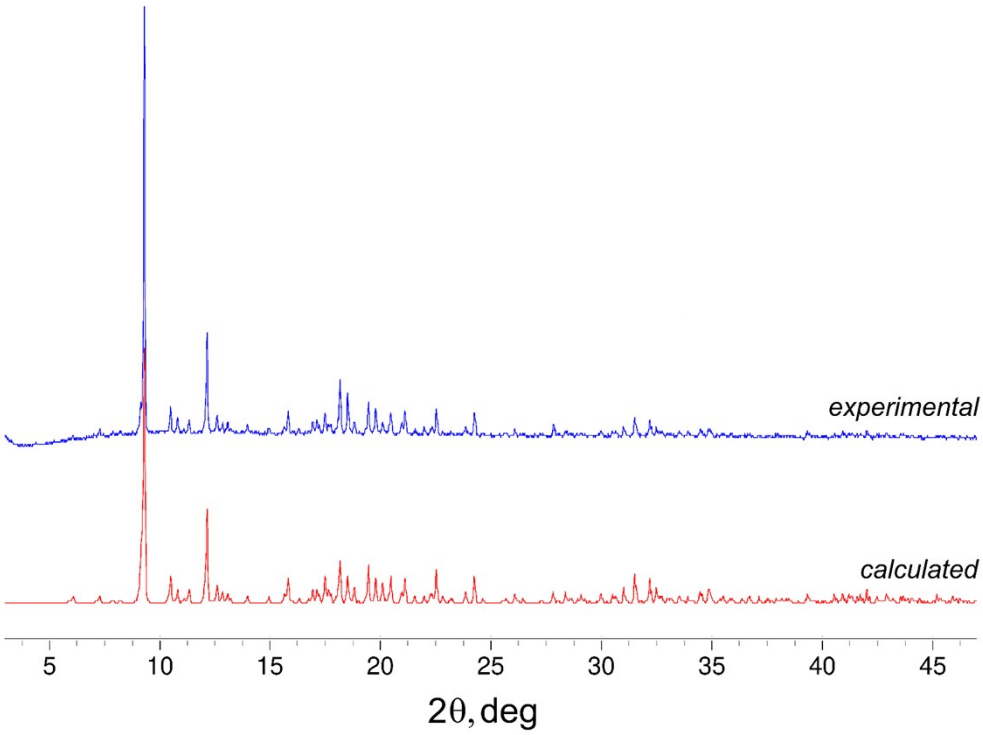



**Fig. S3.** The experimental PXRD pattern for $\mathbf{1}_{\mathbf{Tb}}$ measured at 295 K and its comparison with calculated data for $\mathbf{1}_{\mathbf{Tb}}$.

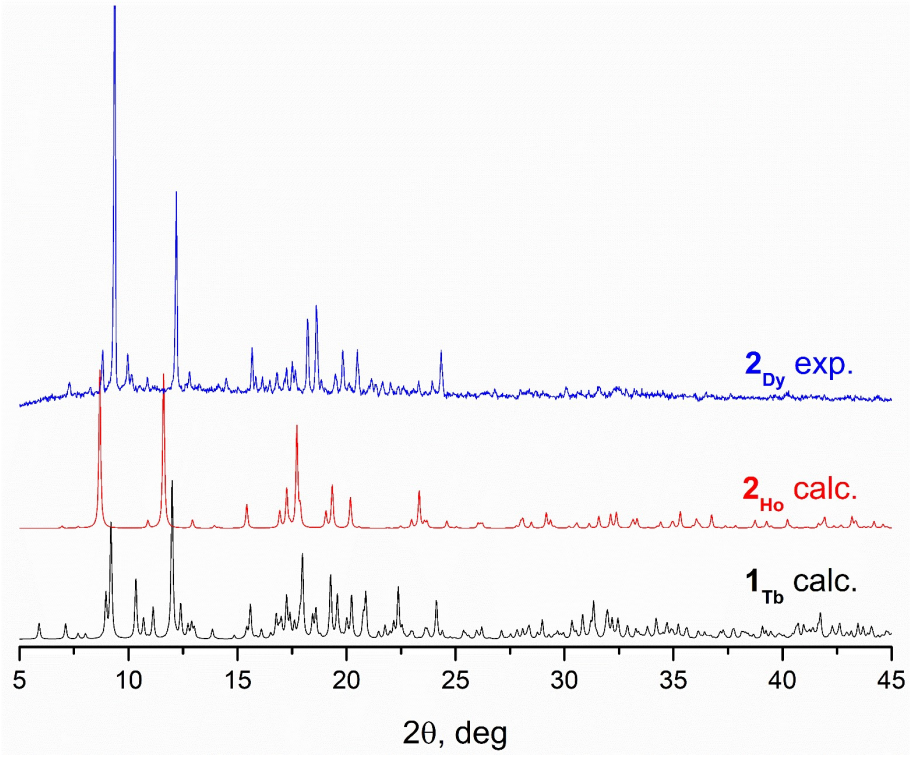



**Fig. S4.** The experimental PXRD pattern for $\mathbf{2}_{\mathbf{Dy}}$ measured at 295 K and its comparison with data calculated from single-crystal XRD for $\mathbf{1}_{\mathbf{Tb}}$ and $\mathbf{2}_{\mathbf{Ho}}$.

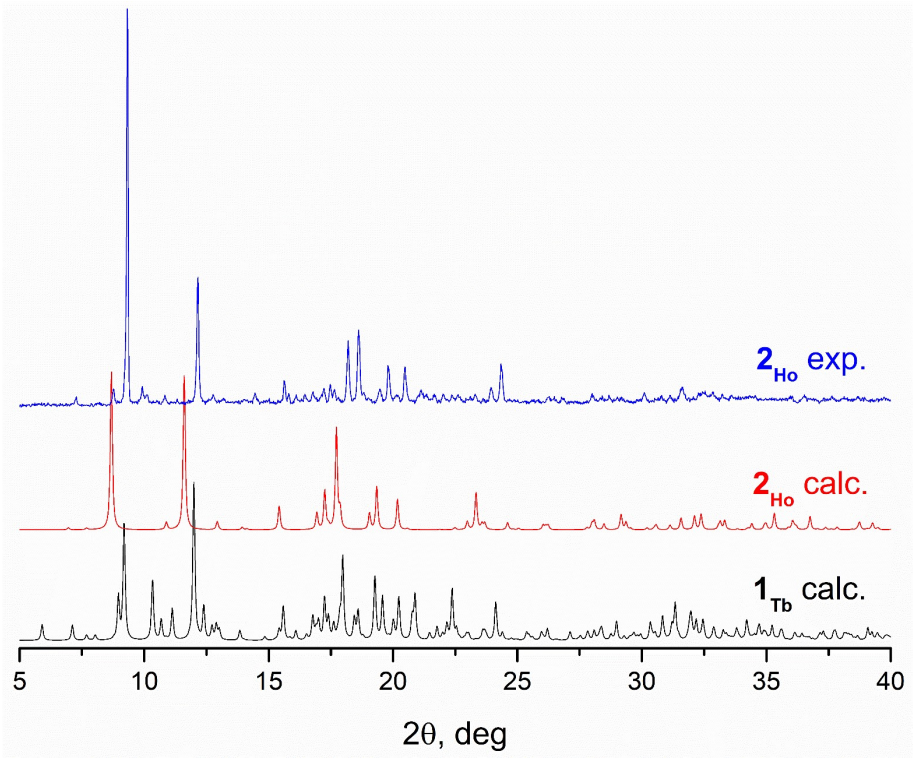



**Fig. S5.** The experimental powder XRD pattern for $\mathbf{2_{Ho}}$ measured at 295 K and its comparison with data calculated from single-crystal XRD for $\mathbf{1_{Tb}}$ and $\mathbf{2_{Ho}}$.

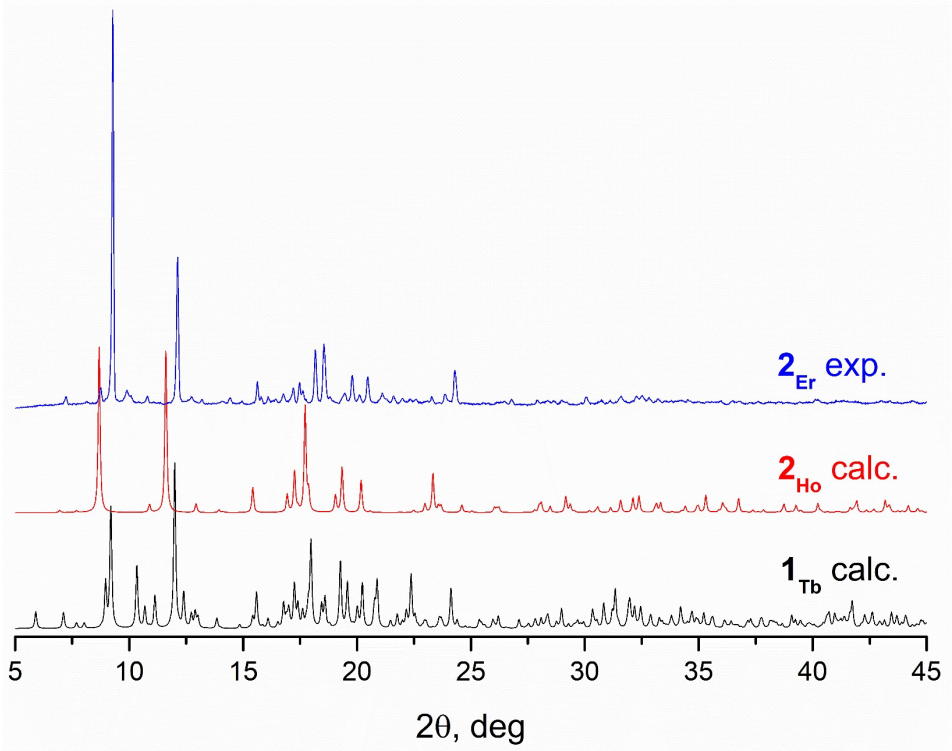



**Fig. S6.** The experimental powder XRD pattern for $\mathbf{2_{Er}}$ measured at 295 K and its comparison with data calculated from single-crystal XRD for $\mathbf{1_{Tb}}$ and $\mathbf{2_{Ho}}$.

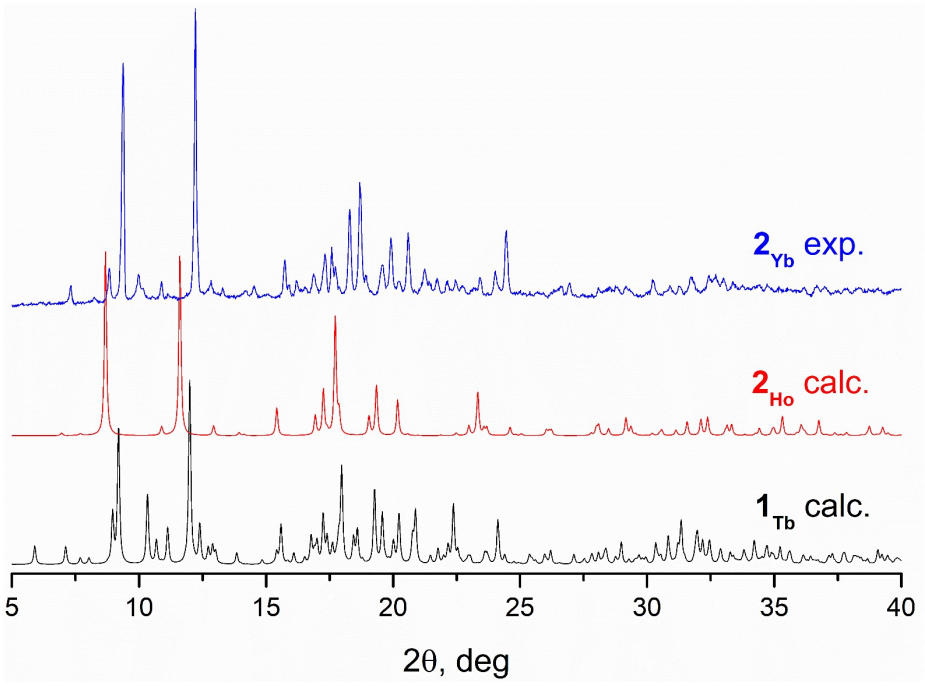



**Fig. S7.** The experimental powder XRD pattern for $\mathbf{2_{Yb}}$ measured at 295 K and its comparison with data calculated from single-crystal XRD for $\mathbf{1_{Tb}}$ and $\mathbf{2_{Ho}}$.

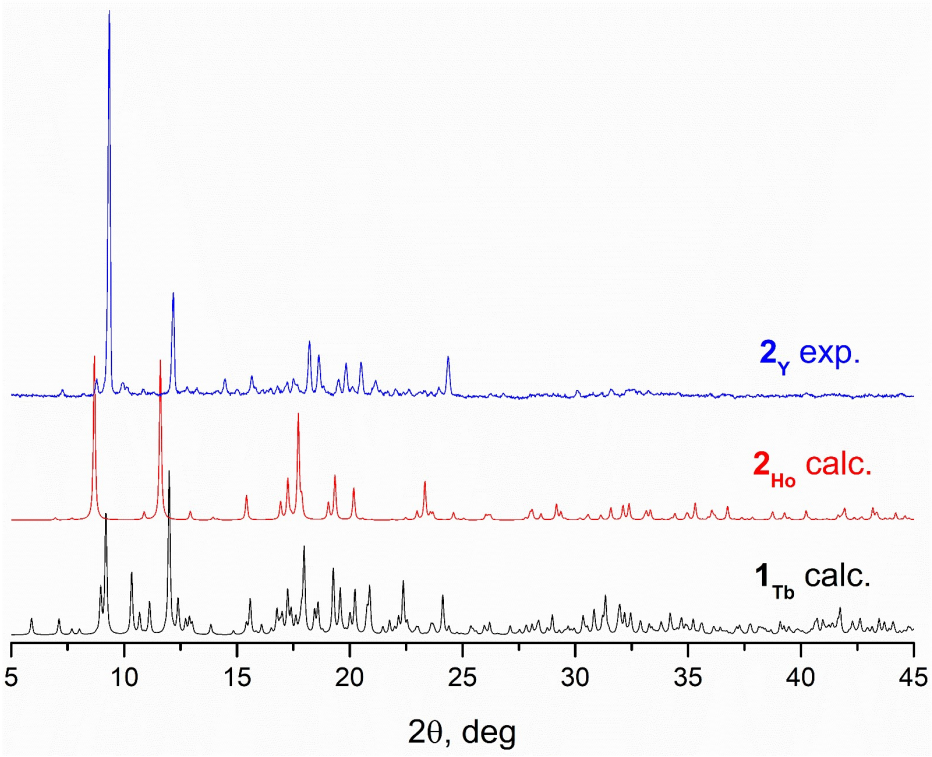



**Fig. S8.** The experimental powder XRD pattern for $\mathbf{2_{Y}}$ measured at 295 K and its comparison with data calculated from single-crystal XRD for $\mathbf{1_{Tb}}$ and $\mathbf{2_{Ho}}$.

## II. The description of crystal structures

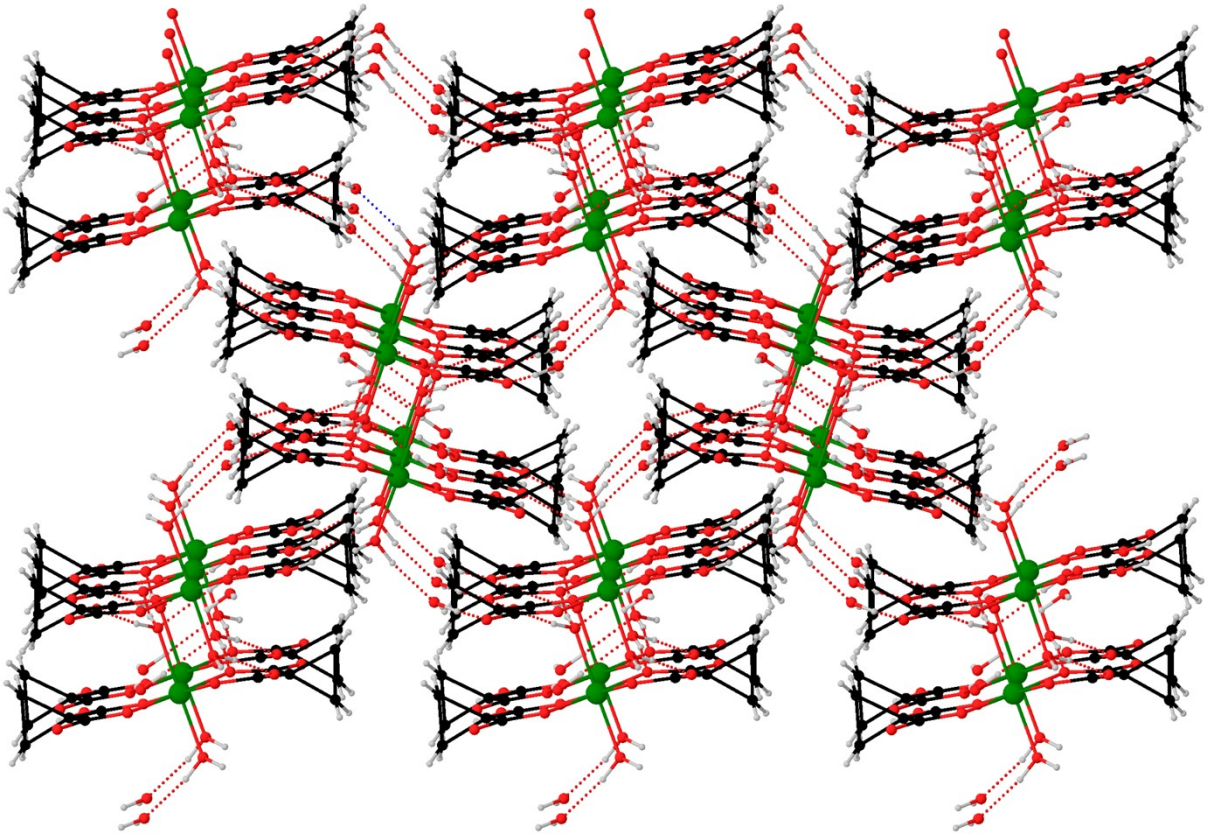


**Fig. S9.** The fragment of crystal packing of compound **3**.

**Table S1.** Continuous shape measures (CShM) for $LnO_8$ coordination polyhedra in compounds $\mathbf{1}_{Eu}$, $\mathbf{1}_{Gd}$, $\mathbf{1}_{Tb}$. The lowest SHAPE values are shown highlighted indicating best fits.

| **Structure, Ln** | **SAPR-8** | **TDD-8** | **JBTPR-8** | **BTPR-8** | **JSD-8** |
|---|---|---|---|---|---|
| $\mathbf{1}_{Eu}$, **Eu1** | 2.378 | 1.149 | 1.627 | **0.952** | 3.224 |
| $\mathbf{1}_{Eu}$, **Eu2** | **0.773** | 1.040 | 1.890 | 1.325 | 3.488 |
| $\mathbf{1}_{Gd}$, **Gd1** | 2.290 | 1.099 | 1.655 | **0.948** | 3.261 |
| $\mathbf{1}_{Gd}$, **Gd2** | **0.761** | 1.076 | 1.860 | 1.313 | 3.499 |
| $\mathbf{1}_{Tb}$, **Tb1** | 2.238 | 1.126 | 1.674 | **0.955** | 3.359 |
| $\mathbf{1}_{Tb}$, **Tb2** | **0.670** | 1.151 | 1.877 | 1.336 | 3.558 |

*Codes*:
SAPR-8 (D4d) Square antiprism;
TDD-8 (D2d) Triangular dodecahedron;
JBTPR-8 (C2v) Biaugmented trigonal prism J50;
BTPR-8 (C2v) Biaugmented trigonal prism;
JSD-8 (D2d) Snub diphenoid J84.

**Table S2.** Selected bond angles $\omega$ (deg.) for $\mathbf{1_{Eu}}$.

| Angle | $\omega$ | Angle | $\omega$ |
|---|---|---|---|
| O7A–Eu1–O11A$^{(i)}$ | 87.63(12) | O3A–Eu2–O8A$^{(i)}$ | 73.01(12) |
| O7A–Eu1–O1 | 73.73(12) | O3A–Eu2–O3B | 74.76(12) |
| O7A–Eu1–O2 | 80.84(12) | O3A–Eu2–O12B$^{(iii)}$ | 111.71(12) |
| O7A–Eu1–O3 | 143.51(11) | O3A–Eu2–O6 | 74.81(12) |
| O7A–Eu1–O4 | 87.53(12) | O3A–Eu2–O7 | 142.23(12) |
| O7A–Eu1–O5 | 74.01(11) | O3A–Eu2–O8 | 143.30(13) |
| O11Ai–Eu1–O5 | 69.74(13) | O3A–Eu2–O9 | 85.70(13) |
| O11B$^{(ii)}$–Eu1–O7A | 146.20(12) | O8A$^{(i)}$–Eu2–O6 | 135.69(12) |
| O11B$^{(ii)}$–Eu1–O11A$^{(i)}$ | 112.49(12) | O8A$^{(i)}$–Eu2–O8 | 74.45(12) |
| O11B$^{(ii)}$–Eu1–O1 | 73.96(12) | O8A$^{(i)}$–Eu2–O9 | 79.39(12) |
| O11B$^{(ii)}$–Eu1–O2 | 80.99(12) | O3B–Eu2–O8Ai | 123.50(12) |
| O11B$^{(ii)}$–Eu1–O3 | 69.84(12) | O3B–Eu2–O12B$^{(iii)}$ | 72.53(12) |
| O11B$^{(ii)}$–Eu1–O4 | 91.54(13) | O3B–Eu2–O6 | 74.71(13) |
| O11B$^{(ii)}$–Eu1–O5 | 137.42(12) | O3B–Eu2–O8 | 139.23(12) |
| O1–Eu1–O11A$^{(i)}$ | 141.85(12) | O3B–Eu2–O9 | 141.79(12) |
| O1–Eu1–O5 | 132.09(12) | O12B$^{(iii)}$–Eu2–O8Ai | 78.09(12) |
| O2–Eu1–O11A$^{(i)}$ | 70.38(11) | O12B$^{(iii)}$–Eu2–O6 | 143.09(13) |
| O2–Eu1–O1 | 73.91(12) | O12B$^{(iii)}$–Eu2–O8 | 77.20(12) |
| O2–Eu1–O3 | 122.32(12) | O12B$^{(iii)}$–Eu2–O9 | 145.67(12) |
| O2–Eu1–O5 | 133.18(12) | O7–Eu2–O8Ai | 144.74(13) |
| O3–Eu1–O11A$^{(i)}$ | 76.49(11) | O7–Eu2–O3B | 78.06(12) |
| O3–Eu1–O1 | 136.18(12) | O7–Eu2–O12B$^{(iii)}$ | 83.91(13) |
| O3–Eu1–O5 | 69.70(11) | O7–Eu2–O6 | 73.06(13) |
| O4–Eu1–O11A$^{(i)}$ | 141.86(13) | O7–Eu2–O8 | 72.10(12) |
| O4–Eu1–O1 | 71.59(13) | O7–Eu2–O9 | 100.38(13) |
| O4–Eu1–O2 | 145.44(12) | O8–Eu2–O6 | 120.27(12) |
| O4–Eu1–O3 | 85.39(13) | O8–Eu2–O9 | 72.00(12) |
| O4–Eu1–O5 | 72.55(13) | O9–Eu2–O6 | 68.54(12) |

Symmetry codes: (i) x-1/2, -y+1/2, -z+1/4; (ii) -y+1, -x+1, -z+1/2; (iii) x-1/2, -y+3/2, -z+1/4.

**Table S3.** Selected bond angles $\omega$ (deg.) for $\mathbf{1_{Gd}}$.

| Angle | $\omega$ | Angle | $\omega$ |
|---|---|---|---|
| O1–Gd1–O5 | 131.53(19) | O3A–Gd2–O3B | 111.68(18) |
| O1–Gd1–O11A$^{(i)}$ | 142.03(17) | O3A–Gd2–O6 | 142.00(18) |
| O2–Gd1–O1 | 74.38(17) | O3A–Gd2–O7 | 143.20(19) |
| O2–Gd1–O3 | 146.34(19) | O3A–Gd2–O8A$^{(iii)}$ | 73.01(18) |
| O2–Gd1–O4 | 122.46(18) | O3A–Gd2–O8 | 85.28(19) |
| O2–Gd1–O5 | 133.49(18) | O3A–Gd2–O9 | 74.93(17) |
| O2–Gd1–O11A$^{(i)}$ | 70.14(17) | O3A–Gd2–O12B$^{(iv)}$ | 74.57(17) |
| O3–Gd1–O1 | 72.00(19) | O3B–Gd2–O7 | 77.57(18) |
| O3–Gd1–O4 | 84.37(19) | O3B–Gd2–O8A$^{(iii)}$ | 78.04(18) |
| O3–Gd1–O5 | 71.7(2) | O3B–Gd2–O8 | 146.13(18) |

| | | | |
|---|---|---|---|
| O3–Gd1–O11A$^{(i)}$ | 141.42(19) | O3B–Gd2–O9 | 142.38(18) |
| O4–Gd1–O1 | 136.06(17) | O6–Gd2–O3B | 84.3(2) |
| O4–Gd1–O5 | 69.48(17) | O6–Gd2–O7 | 72.25(18) |
| O4–Gd1–O11A$^{(i)}$ | 76.68(16) | O6–Gd2–O8A$^{(iii)}$ | 144.98(19) |
| O4B–Gd1–O1 | 74.04(17) | O6–Gd2–O8 | 100.29(19) |
| O4B–Gd1–O2 | 80.98(18) | O6–Gd2–O9 | 72.36(19) |
| O4B–Gd1–O3 | 91.45(18) | O7–Gd2–O8 | 72.16(18) |
| O4B–Gd1–O4 | 70.01(17) | O7–Gd2–O9 | 120.30(17) |
| O4B–Gd1–O5 | 137.29(18) | O8A$^{(iii)}$–Gd2–O7 | 74.53(18) |
| O4B–Gd1–O11A$^{(i)}$ | 112.44(17) | O8A$^{(iii)}$–Gd2–O8 | 79.56(18) |
| O7A$^{(ii)}$–Gd1–O1 | 73.49(18) | O8A$^{(iii)}$–Gd2–O9 | 136.30(18) |
| O7A$^{(ii)}$–Gd1–O2 | 80.69(17) | O8–Gd2–O9 | 68.89(18) |
| O7A$^{(ii)}$–Gd1–O3 | 88.17(18) | O12B$^{(iv)}$–Gd2–O3B | 72.37(18) |
| O7A$^{(ii)}$–Gd1–O4 | 143.59(17) | O12B$^{(iv)}$–Gd2–O6 | 78.39(18) |
| O7A$^{(ii)}$–Gd1–O4B | 145.94(18) | O12B$^{(iv)}$–Gd2–O7 | 139.59(18) |
| O7A$^{(ii)}$–Gd1–O5 | 74.33(17) | O12B$^{(iv)}$–Gd2–O8A$^{(iii)}$ | 123.13(18) |
| O7A$^{(ii)}$–Gd1–O11A$^{(i)}$ | 87.6(17) | O12B$^{(iv)}$–Gd2–O8 | 141.49(18) |
| O11A$^{(i)}$–Gd1–O5 | 70.26(19) | O12B$^{(iv)}$–Gd2–O9 | 74.27(18) |

Symmetry code(s): (i) -*y*+1, -*x*+1, -*z*+1/2; (ii) -*y*+3/2, *x*+1/2, *z*-1/4; (iii) -*x*+1/2, *y*+1/2, -*z*+3/4; (iv) -*x*+3/2, *y*-1/2, -*z*+3/4.

**Table S4.** Selected bond angles $\omega$ (deg.) for $\mathbf{1_{Tb}}$.

| Angle | $\omega$ | Angle | $\omega$ |
|---|---|---|---|
| O7A–Tb1–O11A$^{(i)}$ | 87.25(16) | O3A–Tb2–O8A$^{(i)}$ | 73.27(15) |
| O7A–Tb1–O1 | 73.37(16) | O3A–Tb2–O3B | 74.77(15) |
| O7A–Tb1–O2 | 80.88(15) | O3A–Tb2–O12B$^{(iii)}$ | 112.22(15) |
| O7A–Tb1–O3 | 143.72(15) | O3A–Tb2–O6 | 74.77(15) |
| O7A–Tb1–O4 | 88.41(16) | O3A–Tb2–O7 | 142.30(16) |
| O7A–Tb1–O5 | 74.12(15) | O3A–Tb2–O8 | 142.93(16) |
| O11A$^{(i)}$–Tb1–O4 | 140.53(17) | O3A–Tb2–O9 | 84.49(16) |
| O11A$^{(i)}$–Tb1–O5 | 69.78(17) | O8Ai–Tb2–O6 | 136.37(15) |
| O11B$^{(ii)}$–Tb1–O7A | 145.95(15) | O8Ai–Tb2–O8 | 74.35(16) |
| O11B$^{(ii)}$–Tb1–O11A$^{(i)}$ | 112.99(16) | O8Ai–Tb2–O9 | 79.37(15) |
| O11B$^{(ii)}$–Tb1–O1 | 74.13(16) | O3B–Tb2–O8A$^{(i)}$ | 123.14(15) |
| O11B$^{(ii)}$–Tb1–O2 | 80.77(15) | O3B–Tb2–O12B$^{(iii)}$ | 72.76(15) |
| O11B$^{(ii)}$–Tb1–O3 | 69.95(15) | O3B–Tb2–O6 | 74.55(16) |
| O11B$^{(ii)}$–Tb1–O4 | 91.53(16) | O3B–Tb2–O8 | 139.83(15) |
| O11B$^{(ii)}$–Tb1–O5 | 137.48(16) | O3B–Tb2–O9 | 141.39(16) |
| O1–Tb1–O11A$^{(i)}$ | 141.89(15) | O12B$^{(iii)}$–Tb2–O8A$^{(i)}$ | 77.64(15) |
| O1–Tb1–O4 | 72.77(16) | O12B$^{(iii)}$–Tb2–O6 | 142.94(16) |
| O1–Tb1–O5 | 131.49(17) | O12B$^{(iii)}$–Tb2–O8 | 77.46(15) |
| O2–Tb1–O11A$^{(i)}$ | 70.53(15) | O12B$^{(iii)}$–Tb2–O9 | 145.85(15) |
| O2–Tb1–O1 | 74.13(15) | O7–Tb2–O8A$^{(i)}$ | 144.40(16) |
| O2–Tb1–O3 | 121.78(16) | O7–Tb2–O3B | 78.17(15) |
| O2–Tb1–O4 | 146.87(16) | O7–Tb2–O12B$^{(iii)}$ | 83.56(17) |

| | | | |
|---|---|---|---|
| O2–Tb1–O5 | 133.56(16) | O7–Tb2–O6 | 73.04(16) |
| O3–Tb1–O11A$^{(i)}$ | 76.36(15) | O7–Tb2–O8 | 72.20(16) |
| O3–Tb1–O1 | 136.56(15) | O7–Tb2–O9 | 101.40(17) |
| O3–Tb1–O4 | 84.47(16) | O8–Tb2–O6 | 119.92(16) |
| O3–Tb1–O5 | 69.88(16) | O8–Tb2–O9 | 72.21(15) |
| O4–Tb1–O5 | 71.30(18) | O9–Tb2–O6 | 68.68(16) |

Symmetry code(s): (i) *x*+1/2, -*y*-1/2, -*z*-1/4; (ii) -*y*-1, -*x*-1, -*z*-1/2; (iii) *x*+1/2, -*y*-3/2, -*z*-1/4.

**Table S5.** Hydrogen bond parameters in structure $\mathbf{1_{Eu}}$.

| Fragment D–H···A | Distance/ Å | | | D–H···A /° |
|---|---|---|---|---|
| | D–H | H···A | D···A | |
| O1–H1A···O12A$^{(i)}$ | 0.98 | 1.76 | 2.729(5) | 167 |
| O1–H1B···O2S$^{(i)}$ | 0.88 | 1.79 | 2.651(5) | 168 |
| O2–H2A···O2S$^{(i)}$ | 0.98 | 1.86 | 2.721(5) | 145 |
| O2–H2B···O4B$^{(ii)}$ | 0.85 | 1.91 | 2.741(5) | 166 |
| O3–H3A···O5 | 0.98 | 2.38 | 2.787(5) | 104 |
| O3–H3A···O9 | 0.98 | 2.17 | 3.151(5) | 179 |
| O3–H3B···O6S$^{(i)}$ | 0.98 | 1.68 | 2.660(5) | 180 |
| O4–H4A···O1S | 0.98 | 1.79 | 2.771(5) | 179 |
| O4–H4B···O4S$^{(i)}$ | 0.80 | 1.93 | 2.719(5) | 167 |
| O5–H5A···O5A | 0.84 | 1.94 | 2.749(4) | 162 |
| O5–H5A···O7A | 0.84 | 2.57 | 2.918(5) | 106 |
| O5–H5B···O9 | 0.86 | 1.97 | 2.822(5) | 175 |
| O6–H6A···O4S | 0.84 | 1.94 | 2.749(5) | 163 |
| O6–H6A···O7 | 0.84 | 2.54 | 2.887(5) | 106 |
| O6–H6B···O1A | 0.86 | 2.09 | 2.866(4) | 151 |
| O7–H7A···O1B | 0.98 | 1.81 | 2.788(4) | 180 |
| O7–H7A···O3B | 0.98 | 2.39 | 2.989(5) | 119 |
| O7–H7B···O3S | 0.98 | 1.65 | 2.630(6) | 179 |
| O8–H8A···O5S | 0.84 | 1.87 | 2.703(6) | 176 |
| O8–H8A···O9 | 0.84 | 2.55 | 2.870(5) | 104 |
| O8–H8B···O10B$^{(iii)}$ | 0.84 | 1.98 | 2.751(4) | 154 |
| O9–H9A···O5S | 0.98 | 2.54 | 2.872(6) | 100 |
| O9–H9A···O6A$^{(ii)}$ | 0.98 | 2.00 | 2.983(4) | 180 |
| O9–H9A···O8A$^{(ii)}$ | 0.98 | 2.46 | 3.095(5) | 122 |
| O9–H9B···O8S$^{(i)}$ | 0.98 | 1.96 | 2.919(12) | 164 |
| O9–H9B···O8'$^{(i)}$ | 0.98 | 1.77 | 2.683(16) | 154 |
| O1S–H1SA···O12A | 0.89 | 1.93 | 2.808(4) | 166 |
| O1S–H1SB···O12A | 1.15 | 1.75 | 2.808(4) | 150 |
| O2S–H2SA···O8B$^{(iv)}$ | 0.98 | 1.85 | 2.742(5) | 150 |
| O2S–H2SB···O4A$^{(v)}$ | 0.98 | 1.95 | 2.836(5) | 149 |
| O3S–H3SA···O2B$^{(iii)}$ | 0.95 | 2.02 | 2.960(6) | 170 |
| O3S–H3SA···O4B$^{(iii)}$ | 0.95 | 2.50 | 2.996(6) | 113 |
| O3S–H3SB···O7S | 0.98 | 2.49 | 2.942(8) | 108 |

| | | | | |
|---|---|---|---|---|
| O3S–H3SB···O10S | 0.98 | 2.47 | 2.905(8) | 106' |
| O3S–H3SB···O7' | 0.98 | 2.56 | 3.076(10) | 113 |
| O3S–H3SB···O9S$^{(vi)}$ | 0.98 | 2.30 | 3.243(10) | 161 |
| O3S–H3SB···O9'$^{(vi)}$ | 0.98 | 2.26 | 3.236(16) | 175 |
| O3S–H3SB···O9'$^{(iii)}$ | 0.98 | 2.46 | 2.910(17) | 108 |
| O4S–H4SA···O8S | 0.80 | 1.92 | 2.706(12) | 165 |
| O4S–H4SA···O8' | 0.80 | 2.08 | 2.820(15) | 153 |
| O4S–H4SB···O1B | 0.80 | 2.47 | 3.123(5) | 139 |
| O4S–H4SB···O9B | 0.80 | 2.17 | 2.859(4) | 144 |
| O5S–H5SA···O2A$^{(ii)}$ | 0.98 | 1.97 | 2.798(6) | 140 |
| O5S–H5SB···O7S$^{(i)}$ | 0.95 | 1.88 | 2.685(8) | 140 |
| O5S–H5SB···O7'$^{(i)}$ | 0.95 | 1.78 | 2.694(9) | 161 |
| O6S–H6SA···O5B | 0.98 | 1.82 | 2.797(5) | 172 |
| O6S–H6SB···O4A$^{(vii)}$ | 0.98 | 1.97 | 2.852(6) | 148 |
| O7S–H7SA···O7B | 1.09 | 1.76 | 2.828(8) | 163 |
| O7S–H7SB···O6S | 0.95 | 2.22 | 3.168(8) | 178 |
| O8S–H8SA···O7S | 0.87 | 1.94 | 2.715(15) | 148 |
| O8S–H8SA···O10S | 0.87 | 1.96 | 2.391(16) | 109 |
| O8S–H8SA···O7' | 0.87 | 2.58 | 3.360(17) | 149 |
| O8S–H8SB···O8S$^{(i)}$ | 0.87 | 2.21 | 3.042(17) | 160 |
| O9S–H9SA···O8B | 0.98 | 1.82 | 2.774(10) | 164 |
| O9S–H9SB···O3S$^{(viii)}$ | 0.95 | 2.29 | 3.243(10) | 178 |
| O9S–H9SB···O7'$^{(viii)}$ | 0.95 | 2.58 | 2.951(16) | 104 |
| O9S–H9SB···O9'$^{(ix)}$ | 0.95 | 2.47 | 2.854(17) | 104 |
| C9B–H9BB···O2B$^{(iii)}$ | 0.99 | 2.55 | 3.412(6) | 146 |

Symmetry codes: (i) 1–y, 1–x, 1/2–z; (ii) –1/2+x, 1/2–y, 1/4–z; (iii) –1/2+x ,3/2–y, 1/4–z; (iv) 1/2+x, 3/2–y, 1/4–z; (v) 1/2+x, 1/2–y, 1/4–z; (vi) –1/2+y, 3/2–x, 1/4+z; (vii) 1/2+y, 3/2–x, 1/4+z; (viii) 3/2–y, 1/2+x, –1/4+z; (ix) y, x, –z.

**Table S6.** Hydrogen bond parameters in structure $\mathbf{1_{Gd}}$.

| Fragment D–H···A | Distance/ Å | | | D–H···A /° |
|---|---|---|---|---|
| | D–H | H···A | D···A | |
| O1–H1A···O2 | 0.87 | 2.55 | 2.886(7) | 104 |
| O1–H1A···O5S$^{(i)}$ | 0.87 | 1.79 | 2.659(7) | 180 |
| O1–H1B···O12A$^{(ii)}$ | 0.87 | 1.91 | 2.728(7) | 156 |
| O2–H2A···O11B$^{(iii)}$ | 0.98 | 1.80 | 2.738(8) | 158 |
| O2–H2B···O5S$^{(i)}$ | 0.98 | 1.79 | 2.729(8) | 158 |
| O3–H3A···O6S$^{(ii)}$ | 0.87 | 1.79 | 2.653(8) | 173 |
| O3–H3B···O1 | 0.87 | 2.50 | 2.813(7) | 102 |
| O3–H3B···O1S$^{(iv)}$ | 0.87 | 2.13 | 2.766(8) | 129 |
| O4–H4A···O4B | 0.87 | 2.35 | 2.734(7) | 107 |
| O4–H4A···O4S | 0.87 | 1.90 | 2.665(8) | 147 |
| O4–H4B···O9A$^{(v)}$ | 0.87 | 1.92 | 2.710(6) | 150 |
| O5–H5A···O5A$^{(iv)}$ | 0.87 | 1.87 | 2.742(8) | 179 |
| O5–H5A···O7A$^{(iv)}$ | 0.87 | 2.38 | 2.909(8) | 119 |

| | | | | |
|---|---|---|---|---|
| O5–H5B···O8$^{(iv)}$ | 0.87 | 2.26 | 2.811(8) | 122 |
| O6–H6A···O2S | 0.87 | 1.80 | 2.643(8) | 162 |
| O6–H6A···O7 | 0.87 | 2.45 | 2.825(7) | 107 |
| O6–H6B···O10B$^{(i)}$ | 0.87 | 2.17 | 2.789(7) | 127 |
| O7–H7A···O3S | 0.96 | 1.82 | 2.701(9) | 150 |
| O7–H7B···O1B | 0.79 | 2.00 | 2.754(8) | 161 |
| O8–H8A···O8S | 0.87 | 1.95 | 2.805(10) | 165 |
| O8–H8B···O3S | 0.87 | 2.16 | 2.863(8) | 138 |
| O8–H8B···O6A$^{(vi)}$ | 0.87 | 2.30 | 2.983(7) | 135 |
| O9–H9A···O1A | 0.98 | 2.03 | 2.861(7) | 140 |
| O9–H9B···O6S | 0.98 | 1.81 | 2.753(8) | 160 |
| O1S–H1SA···O12A | 0.88 | 2.14 | 2.814(7) | 133 |
| O1S–H1SB···O12A$^{(vii)}$ | 0.88 | 2.14 | 2.814(7) | 133 |
| O2S–H2SA···O7S | 0.82 | 2.16 | 2.962(10) | 166 |
| O2S–H2SA···O8S' | 0.82 | 2.60 | 2.936(13) | 106 |
| O2S–H2SB···O8S' | 0.87 | 2.56 | 2.936(13) | 107 |
| O2S–H2SB···O9S' | 0.87 | 2.15 | 2.99(3) | 163 |
| O3S–H3SA···O2A$^{(vi)}$ | 0.87 | 1.95 | 2.803(8) | 166 |
| O3S–H3SA···O6A$^{(vi)}$ | 0.87 | 2.47 | 2.965(8) | 117 |
| O3S–H3SB···O5S | 0.87 | 2.41 | 3.209(8) | 152 |
| O3S–H3SB···O7S$^{(vii)}$ | 0.87 | 2.23 | 2.675(9) | 112 |
| O4S–H4SA···O2B | 0.87 | 2.57 | 3.304(8) | 143 |
| O4S–H4SA···O6B | 0.87 | 2.13 | 2.799(7) | 134 |
| O4S–H4SB···O4A$^{(v)}$ | 0.87 | 2.15 | 2.839(8) | 136 |
| O5S–H5SA···O7B | 0.87 | 1.97 | 2.743(9) | 147 |
| O5S–H5SB···O4A$^{(vi)}$ | 0.87 | 2.06 | 2.847(8) | 149 |
| O6S–H6SA···O8S$^{(vii)}$ | 0.87 | 2.00 | 2.727(11) | 140 |
| O6S–H6SB···O2B$^{(i)}$ | 0.87 | 2.04 | 2.879(8) | 162 |
| O7S–H7SA···O4S$^{(i)}$ | 0.99 | 2.33 | 3.164(10) | 141 |
| O7S–H7SA···O8B$^{(i)}$ | 0.99 | 2.11 | 2.765(10) | 122 |
| O7S–H7SB···O8B$^{(i)}$ | 0.99 | 2.28 | 2.765(10) | 109 |
| O8S–H8SA···O8S' | 0.74 | 1.90 | 2.58(2) | 151 |
| O8S–H8SB···O7S$^{(vii)}$ | 0.90 | 1.87 | 2.717(15) | 158 |
| O9S–H9SA···O11B$^{(vii)}$ | 0.98 | 2.04 | 3.00(2) | 163 |
| O9S–H9SB···O7S$^{(vii)}$ | 0.98 | 2.18 | 3.13(2) | 162 |
| C10B–H10D···O9B$^{(ii)}$ | 0.99 | 2.55 | 3.412(9) | 146 |

Symmetry codes: (i) 3/2–x, –1/2+y, 3/4–z; (ii) 3/2–x, 1/2+y, 3/4–z; (iii) 3/2–y, –1/2+x, –1/4+z; (iv) 3/2–y, 1/2+x, –1/4+z; (v) 1–y, 1–x, 1/2–z; (vi) 1/2–x, 1/2+y, 3/4–z; (vii) y, x, 1–z.

**Table S7.** Hydrogen bond parameters in structure $\mathbf{1_{Tb}}$.

| Fragment D–H···A | Distance/ Å | | | D–H···A /° |
|---|---|---|---|---|
| | D–H | H···A | D···A | |
| O1–H1A···O12A$^{(i)}$ | 0.98 | 1.77 | 2.735(7) | 167 |

| | | | | |
|---|---|---|---|---|
| O1–H1B···O2S$^{(i)}$ | 0.88 | 1.80 | 2.667(7) | 167 |
| O1S–H1S···O12A | 0.81 | 2.12 | 2.821(6) | 145 |
| O2–H2A···O7'$^{(ii)}$ | 0.98 | 1.63 | 2.56(9) | 155 |
| O2–H2A···O2S$^{(i)}$ | 0.98 | 1.85 | 2.730(7) | 147 |
| O2–H2B···O4B$^{(iii)}$ | 0.86 | 1.90 | 2.739(7) | 165 |
| O3–H3A···O5 | 0.98 | 2.36 | 2.768(7) | 104 |
| O3–H3A···O9 | 0.98 | 2.18 | 3.158(7) | 179 |
| O3–H3B···O6S$^{(i)}$ | 0.98 | 1.69 | 2.673(8) | 178 |
| O4–H4A···O1S | 0.92 | 1.86 | 2.754(7) | 164 |
| O4–H4B···O4S$^{(i)}$ | 1.04 | 1.69 | 2.635(7) | 148 |
| O5–H5A···O5A | 0.84 | 1.93 | 2.742(6) | 162 |
| O5–H5A···O7A | 0.84 | 2.56 | 2.897(7) | 105 |
| O5–H5B···O9 | 0.86 | 1.97 | 2.824(7) | 176 |
| O6–H6A···O4S | 0.84 | 1.93 | 2.743(7) | 162 |
| O6–H6A···O7 | 0.84 | 2.52 | 2.867(7) | 106 |
| O6–H6B···O1A | 0.86 | 2.08 | 2.870(6) | 151 |
| O7–H7A···O1B | 0.98 | 1.80 | 2.781(7) | 179 |
| O7–H7A···O3B | 0.98 | 2.38 | 2.968(6) | 118 |
| O7–H7B···O3S | 0.98 | 1.66 | 2.640(8) | 177 |
| O8–H8A···O5S | 0.84 | 1.88 | 2.714(8) | 176 |
| O8–H8A···O9 | 0.84 | 2.53 | 2.858(7) | 104 |
| O8–H8B···O10B$^{(iv)}$ | 0.83 | 1.98 | 2.750(6) | 154 |
| O9–H9A···O6A$^{(iii)}$ | 0.98 | 1.98 | 2.954(6) | 180 |
| O9–H9A···O8A$^{(iii)}$ | 0.98 | 2.45 | 3.072(6) | 121 |
| O9–H9B···O8S$^{(i)}$ | 0.98 | 1.99 | 2.941(13) | 164 |
| O9–H9B···O8'$^{(i)}$ | 0.98 | 1.75 | 2.668(16) | 155 |
| O2S–H2SA···O8B$^{(v)}$ | 0.98 | 1.85 | 2.751(7) | 150 |
| O2S–H2SB···O4A$^{(vi)}$ | 0.98 | 1.99 | 2.867(7) | 148 |
| O3S–H3SA···O2B$^{(iv)}$ | 0.95 | 2.01 | 2.949(8) | 169 |
| O3S–H3SA···O4B$^{(iv)}$ | 0.95 | 2.51 | 3.007(8) | 113 |
| O3S–H3SB···O7S | 0.98 | 2.45 | 2.933(10) | 110 |
| O3S–H3SB···O4S' | 0.98 | 2.46 | 2.907(13) | 108 |
| O3S–H3SB···O9S$^{(vii)}$ | 0.98 | 2.32 | 3.260(14) | 160 |
| O3S–H3SB···O9'$^{(vii)}$ | 0.98 | 2.25 | 3.23(2) | 174 |
| O3S–H3SB···O9'$^{(iv)}$ | 0.98 | 2.50 | 2.95(2) | 108 |
| O4S–H4SA···O8S | 0.80 | 1.88 | 2.665(13) | 166 |
| O4S–H4SA···O8' | 0.80 | 2.17 | 2.902(17) | 152 |
| O4S–H4SB···O1B | 0.80 | 2.51 | 3.162(7) | 140 |
| O4S–H4SB···O9B | 0.80 | 2.23 | 2.925(7) | 145 |
| O5S–H5SA···O2A$^{(iii)}$ | 0.98 | 1.97 | 2.803(8) | 141 |
| O5S–H5SB···O7S$^{(i)}$ | 0.95 | 1.85 | 2.689(9) | 146 |
| O5S–H5SB···O7'$^{(i)}$ | 0.95 | 2.28 | 3.16(8) | 154 |
| O6S–H6SA···O5B | 0.98 | 1.83 | 2.807(7) | 172 |
| O6S–H6SB···O4A$^{(viii)}$ | 0.98 | 1.97 | 2.854(8) | 149 |

| | | | | |
|---|---|---|---|---|
| O7S–H7SA···O7B | 0.98 | 1.84 | 2.773(9) | 158 |
| O7S–H7SB···O6S | 0.98 | 2.22 | 3.199(10) | 173 |
| O8S–H8SA···O7S | 0.87 | 2.11 | 2.892(17) | 149 |
| O8S–H8SA···O4S' | 0.87 | 2.00 | 2.44(2) | 110 |
| O8S–H8SB···O8S$^{(i)}$ | 0.87 | 2.22 | 3.05(2) | 159 |
| O9S–H9SA···O8B | 0.98 | 1.82 | 2.778(14) | 165 |
| O9S–H9SB···O3S$^{(ix)}$ | 0.95 | 2.31 | 3.260(14) | 178 |
| O9S–H9SB···O9'$^{(x)}$ | 0.95 | 2.46 | 2.86(2) | 105 |
| C9B–H9BA···O2B$^{(iv)}$ | 0.99 | 2.54 | 3.414(8) | 148 |

Symmetry codes: (i) –1–y, –1–x, –1/2–z; (ii) x, 1+y, z; (iii) 1/2+x, –1/2–y, –1/4–z; (iv) 1/2+x, –3/2–y, –1/4–z; (v) –1/2+x, –3/2–y, –1/4–z; (vi) –1/2+x, –1/2–y, –1/4–z; (vii) 1/2+y, –3/2–x, –1/4+z; (viii) –1/2+y, –3/2–x, –1/4+z; (ix) –3/2–y, –1/2+x, 1/4+z; (x) y, x, –z.

**Table S8.** Hydrogen bond parameters in structure **3**.

| Fragment D–H···A | Distance/ Å | | | D–H···A /° |
|---|---|---|---|---|
| | D–H | H···A | D···A | |
| O1S–H1S'···O10$^{(i)}$ | 0.86 | 1.97 | 2.770(3) | 154 |
| O1S–H1S···O9$^{(ii)}$ | 0.85 | 1.95 | 2.798(3) | 175 |
| O2S–H2S'···O6$^{(iii)}$ | 0.85 | 2.02 | 2.869(3) | 174 |
| O2S–H2S···O1$^{(iv)}$ | 0.89 | 1.83 | 2.706(2) | 169 |
| O5–H5···O7$^{(v)}$ | 0.89 | 1.88 | 2.774(3) | 175 |
| O5–H5'···O1S | 0.87 | 1.74 | 2.604(3) | 171 |
| O6–H6···O4$^{(iii)}$ | 0.83 | 1.94 | 2.765(2) | 170 |
| O6–H6'···O9$^{(vi)}$ | 0.81 | 1.81 | 2.605(2) | 169 |
| O8–H8···O5$^{(i)}$ | 0.95 | 2.39 | 3.341(3) | 180 |

Symmetry codes: (i) 1–x, 1/2+y, 3/2–z; (ii) 2–x, 1/2+y, 3/2–z; (iii) 1–x, 1–y, 1–z; (iv) –1+x, y, z; (v) 2–x, –1/2+y, 3/2–z; (vi) 2–x, 1–y, 1–z.

## III. Magnetic properties

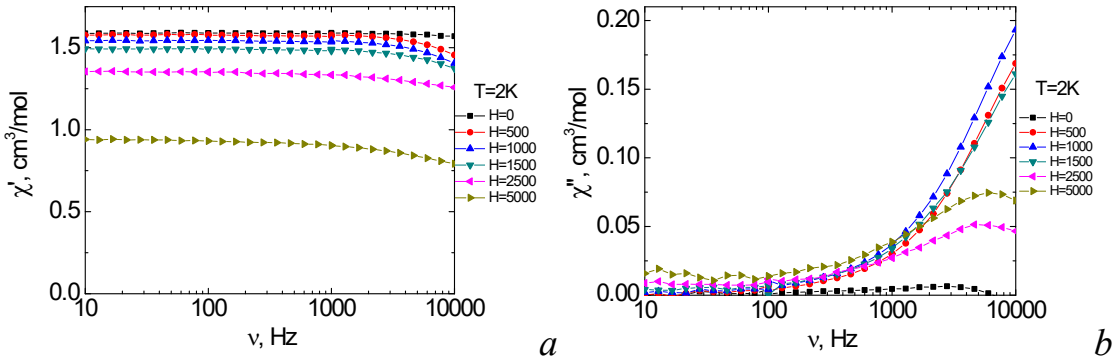



**Fig. S10.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{1}_{\mathbf{Eu}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

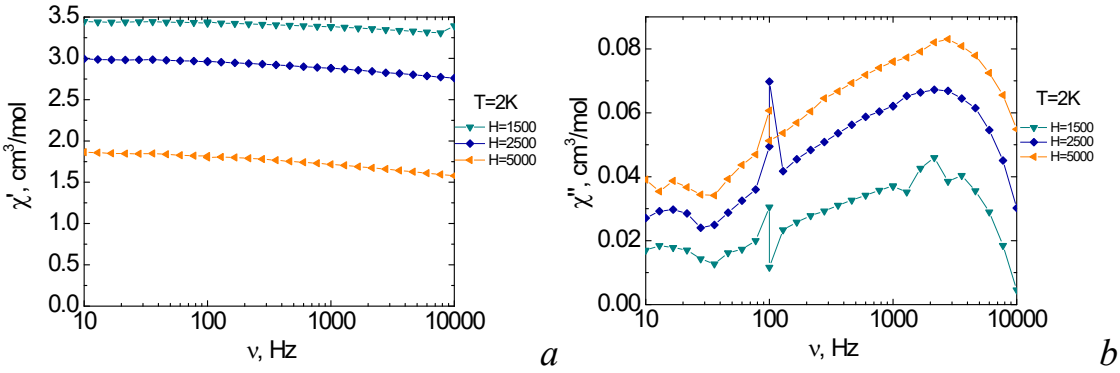



**Fig. S11.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{1}_{\mathbf{Gd}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

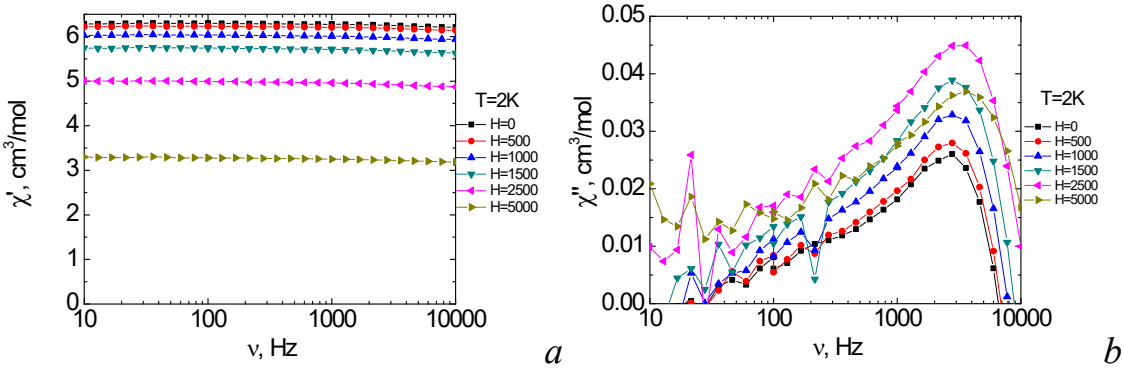



**Fig. S12.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{1}_{\mathbf{Tb}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

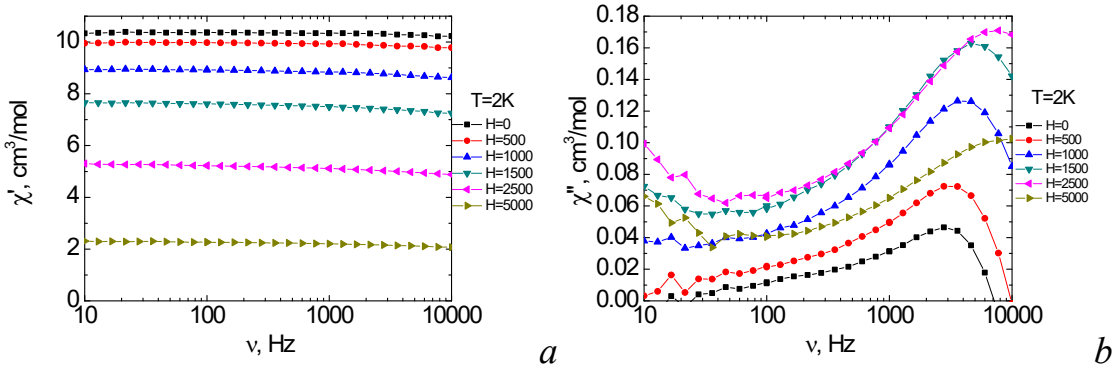



**Fig. S13.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{2_{Dy}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

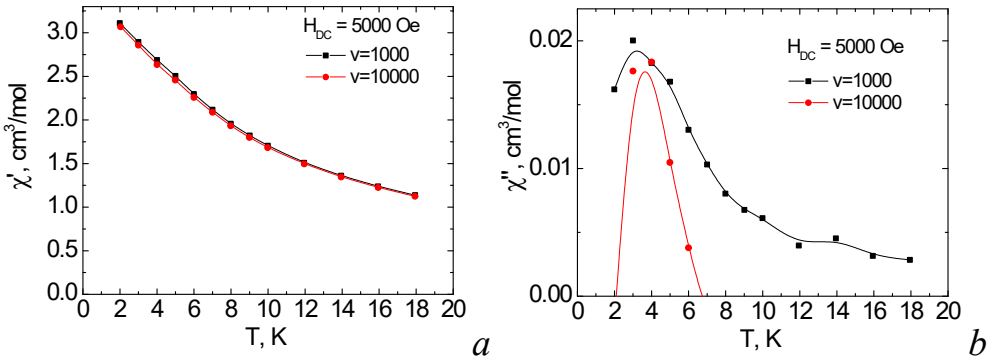



**Fig. S14.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{2_{Ho}}$ under magnetic field H = 5000 Oe under various temperatures. Solid lines are visual guides.

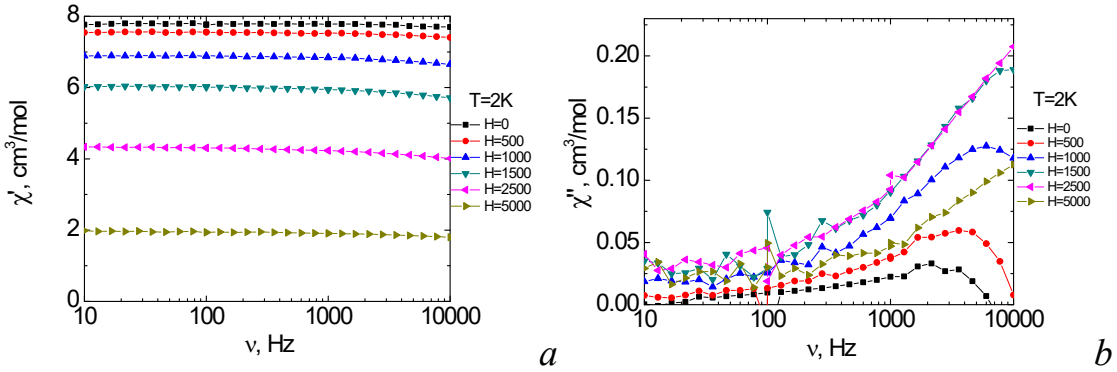



**Fig. S15.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{2_{Er}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

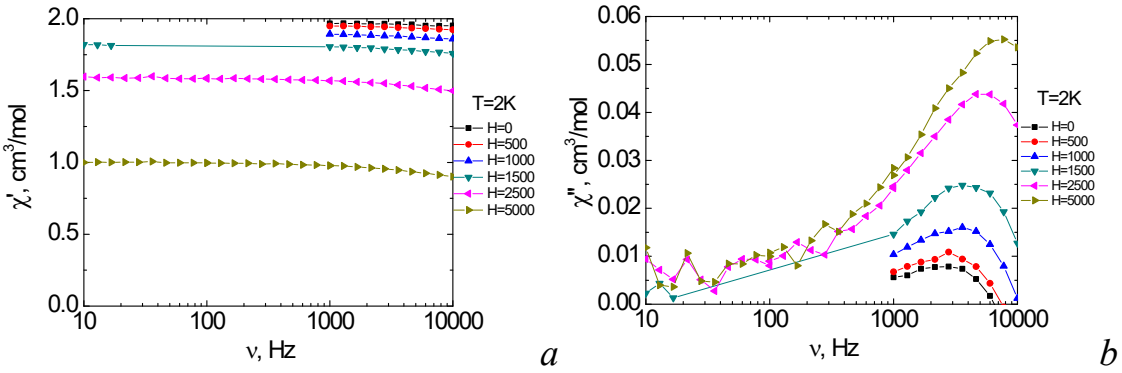



**Fig. S16.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{2_{Yb}}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

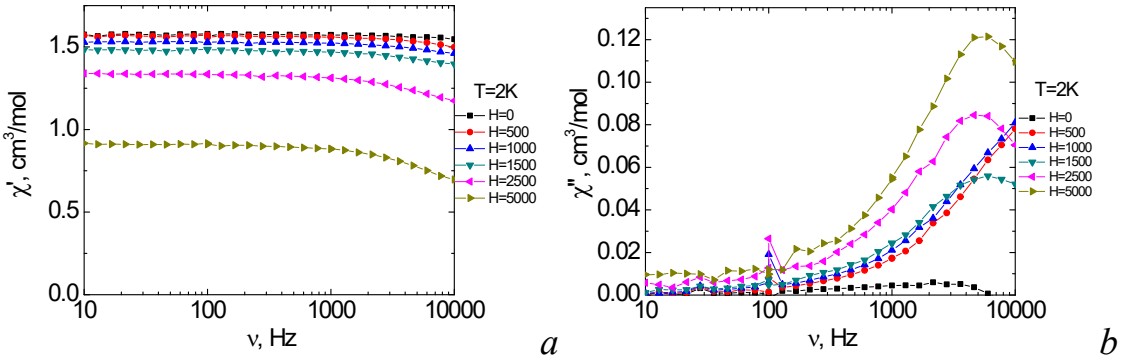



**Fig. S17.** Frequency dependencies of in-phase, χ' (*a*) and out-of-phase, χ'' (*b*) components of dynamic magnetic susceptibility for complex $\mathbf{2_Y}$ at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

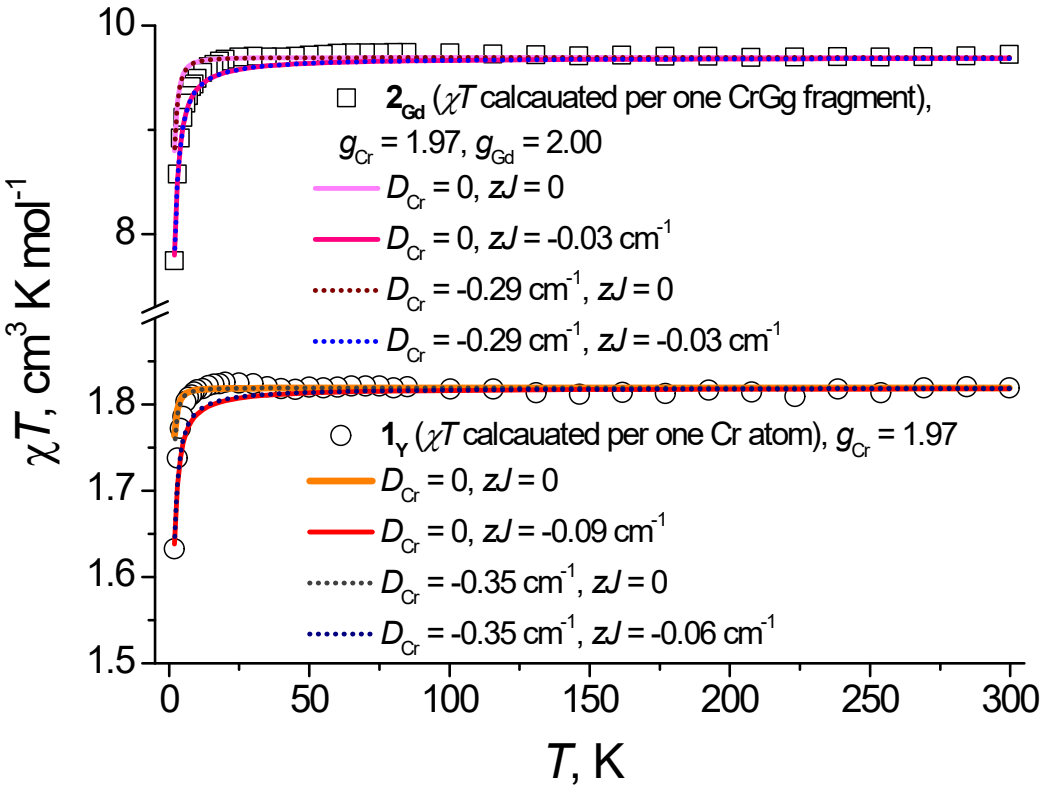



**Fig. S18.** Experimental $\chi T$ vs. $T$ plots and fits (see Table S9 for details) for compounds $\mathbf{2_Y}$ (at the bottom) and $\mathbf{1_{Gd}}$ (at the top) at 2-300 K, $H_{dc}$ = 5000 Oe.

**Table S9.** Best-fit approximation parameters of $\chi T$ vs. $T$ curves for $\mathbf{2_Y}$ and $\mathbf{1_{Gd}}$ ($g$-factors were fixed: $g_{Cr} = 1.97$, $g_{Gd} = 2.00$; $R^2 = \sum[(\chi_M T)_{exp}-(\chi_M T)_{theor}]^2/(\sum(\chi_M T)_{exp}^2)$).

| Fit number | 1 | 2 | 3 | | 4 |
|---|---|---|---|---|---|
| Fit details | $zJ = 0$ | $zJ \neq 0$ | $zJ = 0$ | | $zJ \neq 0$ |
| $\mathbf{2_Y}$ | $D_{Cr} = 0$ | | $D_{Cr} = -1.1$ cm$^{-1}$ | $D_{Cr} = -0.35$ cm$^{-1}$ | |
| | $R^2 = 1.7\cdot10^{-4}$ | $zJ = -0.09$ cm$^{-1}$, $R^2 = 8.9\cdot10^{-5}$ | $R^2 = 6.9\cdot10^{-5}$ | $R^2 = 1.3\cdot10^{-4}$ | $zJ = -0.06$ cm$^{-1}$, $R^2 = 4.4\cdot10^{-5}$ |
| $\mathbf{1_{Gd}}$ | $D_{Cr} = 0$ | | $D_{Cr} = -7.0$ cm$^{-1}$ | $D_{Cr} = -0.29$ cm$^{-1}$ | |
| | $R^2 = 6.4\cdot10^{-4}$ | $zJ = -0.03$ cm$^{-1}$, $R^2 = 6.5\cdot10^{-5}$ | $R^2 = 6.9\cdot10^{-5}$ | $R^2 = 6.3\cdot10^{-4}$ | $zJ = -0.03$ cm$^{-1}$, $R^2 = 6.6\cdot10^{-5}$ |

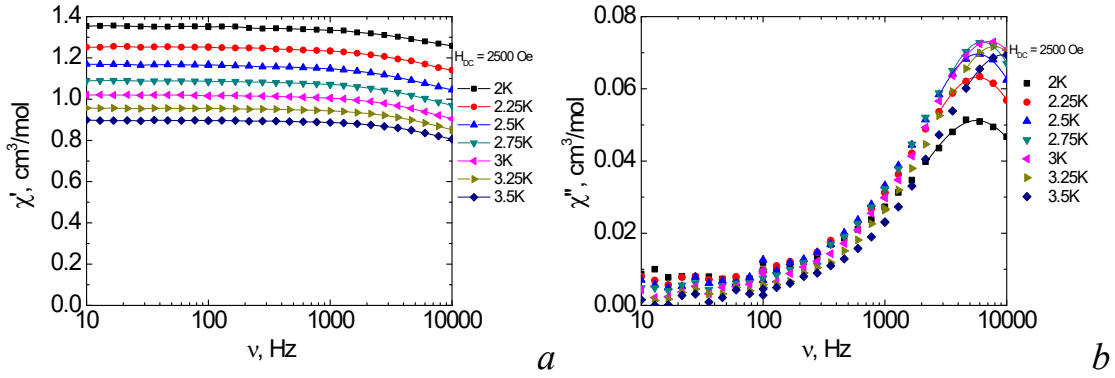



**Fig. S19.** Frequency dependences of the in-phase χ′ (*a*) and out-of-phase χ″ (*b*) components of the *ac* magnetic susceptibility between 2 and 3.5 K for $\mathbf{1_{Eu}}$ in 2500 Oe *dc*-field. Solid lines are visual guides (*a*), fits by the generalized Debye model (*b*).

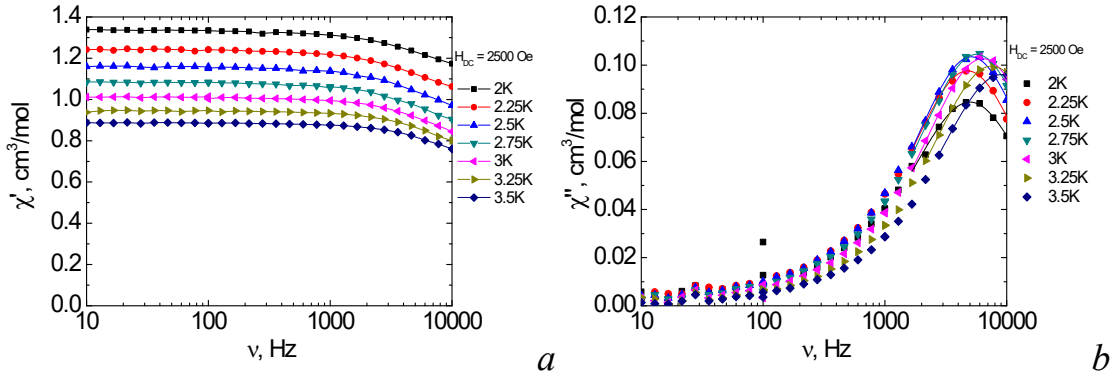



**Fig. S20.** Frequency dependences of the in-phase χ′ (*a*) and out-of-phase χ″ (*b*) components of the *ac* magnetic susceptibility between 2 and 3.5 K for $\mathbf{2_Y}$ in 2500 Oe *dc*-field. Solid lines are visual guides (*a*), fits by the generalized Debye model (*b*).

## IV. Quantum-chemical calculations

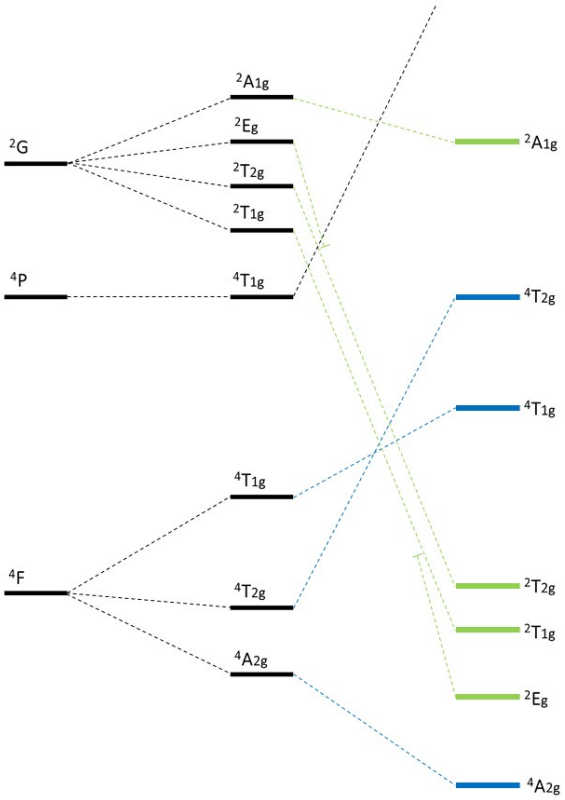



**Fig. S21.** The scheme of splitting of the three main orbital $^4F$ and $^2G$ levels as a result of distortion of the crystal field (relative arrangement of levels, the scale is not respected).

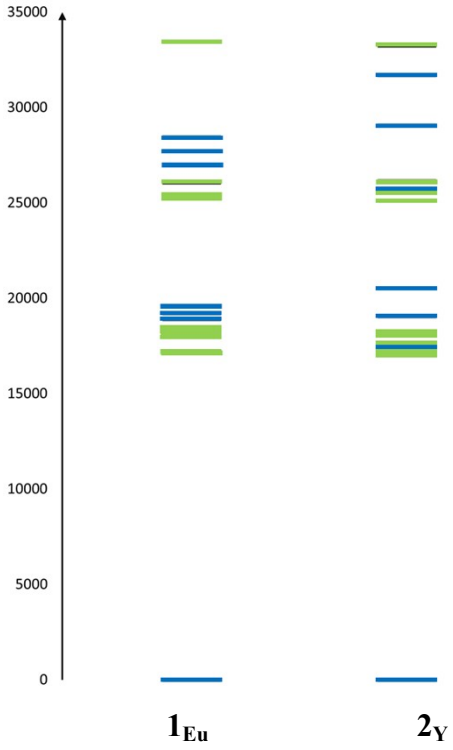



**Fig. S22.** Calculated energies of components of initial states for complexes $\mathbf{1_{Eu}}$ and $\mathbf{2_Y}$. Blue and green levels are orbital quartets and doublets, respectively.

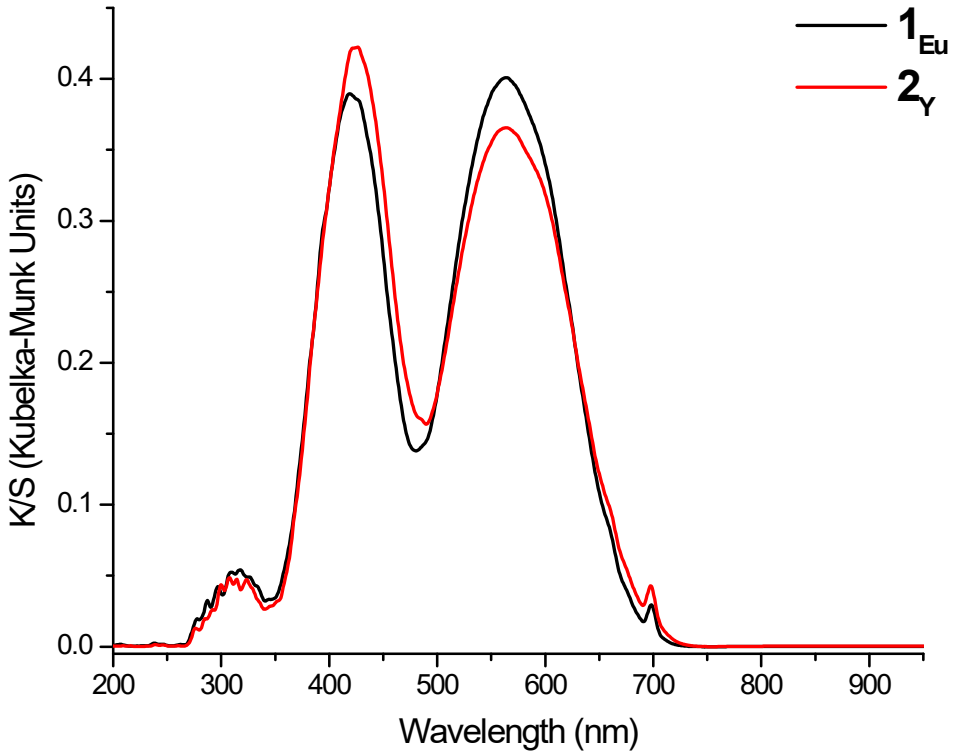



**Fig. S23.** Diffuse reflectance spectra of compounds $\mathbf{1}_{Eu}$ and $\mathbf{1}_{Y}$.

**Table S10.** Calculated energies of the electronic states for $Cr^{3+}$ ions in complexes $\mathbf{1}_{Eu}$ and $\mathbf{2}_{Y}$.

| Term | $\mathbf{1}_{Eu}$ | | $\mathbf{2}_{Y}$ | |
|---|---|---|---|---|
| | **E, cm$^{-1}$** | **λ, nm** | **E, cm$^{-1}$** | **λ, nm** |
| $^4A_{2g}$ | 0 | 0 | 0 | 0 |
| $^2E_g$ | 17189.0<br>17214.3 | 581 | 17032.8<br>17085.0 | 586 |
| $^2T_{1g}$ | 18024.2<br>18289.5<br>18363.1 | 549 | 17621.7<br>18080.3<br>18246.1 | 556 |
| $^4T_{1g}$ | 18904.3<br>19212.3<br>19594.4 | 520 | 17383.2<br>19055.7<br>20518.1 | 527 |
| $^2T_{2g}$ | 25229.1<br>25366.2<br>26076.6 | 391 | 25116.1<br>25608.7<br>26130.5 | 390 |
| $^4T_{2g}$ | 26991.2<br>27711.4<br>28425.5 | 361 | 25668.5<br>29051.5<br>31691.7 | 347 |
| $^2A_{1g}$ | 33446.3 | 299 | 33253.1 | 301 |

**Table S11.** The contribution of levels to the axial and rhombic components of magnetic anisotropy.

| Term | $\mathbf{1}_{Eu}$ | | $\mathbf{2}_{Y}$ | |
|---|---|---|---|---|
| | *D* | *E* | *D* | *E* |
| $^4T_{1g}$ | -0.727<br>0.676<br>-0.055 | 0.135<br>0.188<br>-0.323 | -1.049<br>0.434<br>0.379 | 0.099<br>-0.608<br>0.463 |
| $^2T_{1g}$ | -0.706<br>-0.689<br>1.136 | -0.711<br>0.687<br>-0.002 | -0.637<br>-0.624<br>1.176 | -0.621<br>0.631<br>-0.025 |

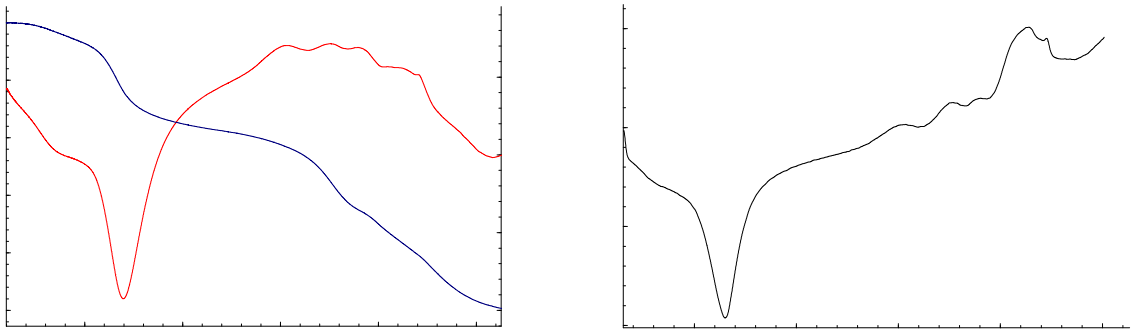
**Table S12.** Calculated parameters of spin Hamiltonian (1).

| Parameter | $\mathbf{1}_{Eu}$ | $\mathbf{2}_{Y}$ |
|---|---|---|
| *D*, $см^{-1}$ | -0.293 | -0.348 |
| *E*/*D* | 0.098 | 0.124 |
| $g_z$ | 1.970 | 1.967 |
| $g_x$ | 1.972 | 1.972 |
| $g_y$ | 1.971 | 1.974 |
| $g_{iso}$ | 1.971 | 1.971 |

**Table S13.** Energies of six lower Kramers doublets.

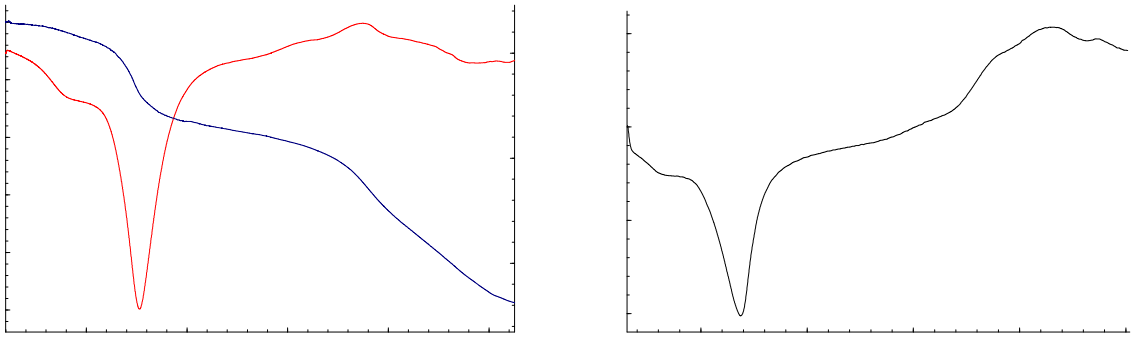
| $\mathbf{1}_{Eu}$ | $\mathbf{2}_{Y}$ |
|---|---|
| 0 | 0 |
| 0.6 | 0.7 |
| 17134.4 | 16894.4 |
| 17170.8 | 17042.1 |
| 17992.1 | 17360.7 |
| 18254.2 | 17478.8 |

## V. Thermal analysis



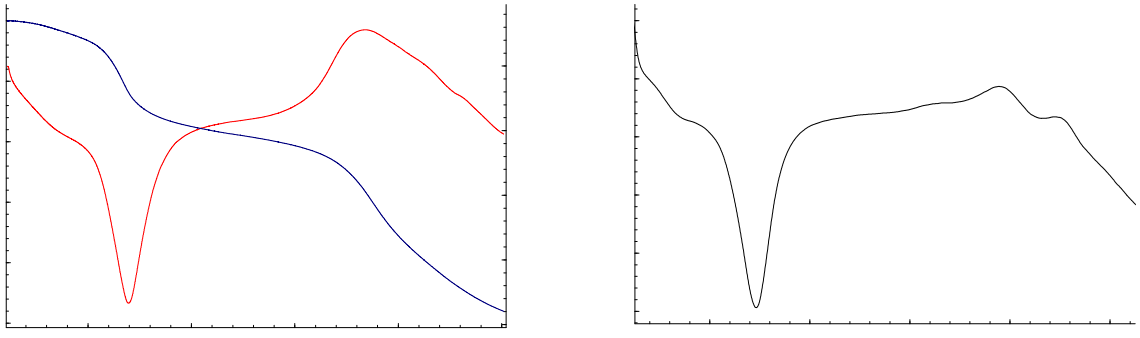
*a* *b*

**Fig. S24.** TGA (blue), DTA (red) (*a*) and DSC (*b*) curves for the thermal decomposition of $\mathbf{1}_{\mathbf{Eu.}}$



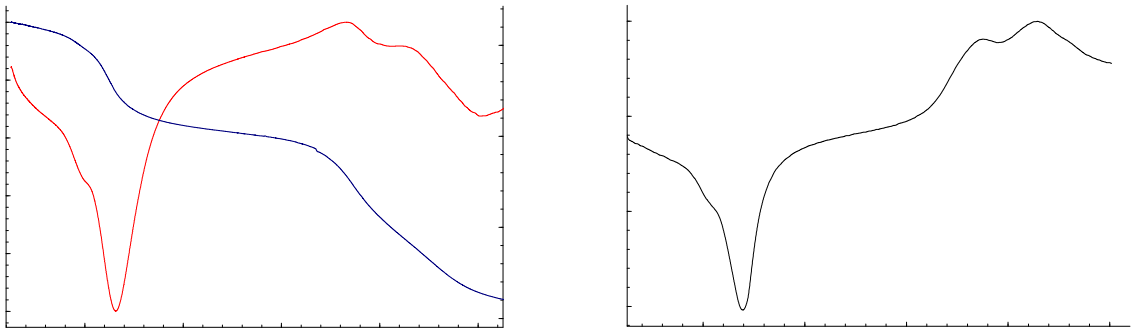
*a* *b*

**Fig. S25.** TGA (blue), DTA (red) (*a*) and DSC (*b*) curves for the thermal decomposition of $\mathbf{1}_{\mathbf{Gd.}}$



*a* *b*

**Fig. S26.** TGA (blue), DTA (red) (*a*) and DSC (*b*) curves for the thermal decomposition of $\mathbf{1}_{\mathbf{Tb.}}$



*a* *b*

**Fig. S27.** TGA (blue), DTA (red) (*a*) and DSC (*b*) curves for the thermal decomposition of **2**$_{Ho}$.

**Table S14.** Characteristics of the solid-phase thermolysis of **1**$_{Eu}$, **1**$_{Gd}$, **1**$_{Tb}$, **2**$_{Ho}$.

| Complex | $t_{onset}$ (I), °C | $t_{onset}$ (II), °C | $t_{onset}$ (III), °C | Δm (I), % | $\Delta m_{expected}$ (I), % | Δm (II), % | Δm (III), % |
|---|---|---|---|---|---|---|---|
| **1**$_{Eu}$ | 28 | 246 | 534.7 | 18.9 | 19.8 | 30.9 | 4.8 |
| **1**$_{Gd}$ | 41 | 283 | 539.2 | 19.4 | 19.7 | 30.8 | 6.1 |
| **1**$_{Tb}$ | 25 | 251 | 529 | 19.1 | 19.6 | 29.1 | 4.9 |
| **2**$_{Ho}$ | 26 | 243.9 | 541.3 | 18.9 | 19.5 | 29.5 | 6.2 |

## VI. X-Ray Crystallography

**Table S15.** Crystallographic parameters and structure refinement statistics for compounds $\mathbf{1_{Eu}}$, $\mathbf{1_{Gd}}$, $\mathbf{1_{Tb}}$, $\mathbf{2_{Ho}}$, and **3**.

| **Parameter** | $\mathbf{1_{Eu}}$ | $\mathbf{1_{Gd}}$ | $\mathbf{1_{Tb}}$ | $\mathbf{2_{Ho}}$ | **3** |
|---|---|---|---|---|---|
| Empirical formula | $C_{30}H_{59}Cr_2Eu_2O_{41.5}$ | $C_{30}H_{59}Cr_2Gd_2O_{41.5}$ | $C_{30}H_{59}Cr_2Tb_2O_{41.5}$ | $C_{30}H_{48}Cr_2Ho_2O_{37}$ | $C_{10}H_{17}CrO_{12}$ |
| Formula weight ($g\cdot mol^{-1}$) | 1491.69 | 1505.61 | 1502.27 | 1434.54 | 381.23 |
| $T$ (K) | 150 | 150 | 150 | 150 | 296 |
| Crystal system | Tetragonal | Tetragonal | Tetragonal | Tetragonal | Monoclinic |
| Space group | $P4_32_12$ | $P4_32_12$ | $P4_12_12$ | $I4$ | $P2_1/c$ |
| $a$ (Å) | 16.2441(3) | 16.2257(6) | 16.2441(3) | 16.2371(6) | 8.3636(4) |
| $b$ (Å) | 16.2441(3) | 16.2257(6) | 16.2441(3) | 16.2371(6) | 12.1817(6) |
| $c$ (Å) | 38.4605(17) | 38.4293(18) | 38.4605(17) | 20.3655(11) | 14.0600(6) |
| β (deg) | 90 | 90 | 90 | 90 | 97.025(2) |
| $V$ (Å$^3$) | 10148.6(6) | 10117.4(9) | 10148.6(6) | 5369.2(5) | 1421.72(12) |
| $Z$ | 8 | 8 | 8 | 4 | 4 |
| $D_{calc}$ ($g\cdot cm^{-3}$) | 1.953 | 1.973 | 1.971 | 1.775 | 1.781 |
| $\theta_{min}$–$\theta_{max}$ (deg) | 2.38−30.50 | 2.38−26.39 | 2.39−30.11 | 2.51–30.41 | 2.45−30.48 |
| μ ($mm^{-1}$) | 2.97 | 3.12 | 3.29 | 3.41 | 0.87 |
| Crystal size (mm) | 0.12×0.11×0.10 | 0.1×0.05×0.05 | 0.11×0.11×0.1 | 0.09×0.08×0.01 | 0.13×0.11×0.10 |
| Number of measured reflections | 105349 | 50195 | 84053 | 20459 | 7680 |
| Number of independent reflections | 13498 | 9940 | 9976 | 5215 | 2749 |
| Number of reflections with $I > 2\sigma(I)$ | 12821 | 9054 | 9384 | 4997 | 2464 |
| $R_{int}$ | 0.048 | 0.069 | 0.059 | 0.113 | 0.022 |
| GOOF | 1.042 | 1.037 | 1.034 | 1.095 | 1.208 |
| $R_1$[a], $wR_2$[b] ($I > 2\sigma(I)$) | 0.024, 0.056 | 0.032, 0.064 | 0.025, 0.055 | 0.0594, 0.1592 | 0.035, 0.096 |
| $R_1$[a], $wR_2$[b] (all data) | 0.027, 0.057 | 0.039, 0.067 | 0.029, 0.057 | 0.0622, 0.1629 | 0.040, 0.099 |
| $T_{min}$, $T_{max}$ | 0.298, 0.381 | 0.586, 0.745 | 0.654, 0.746 | 0.257, 0.381 | 0.323, 0.381 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ ($e$ Å$^{-3}$) | 1.9, −0.69 | 0.69, −0.70 | 0.70, −0.64 | 1.72, −1.08 | 0.50, −0.56 |

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$