

## ELECTRONIC SUPPORTING INFORMATION

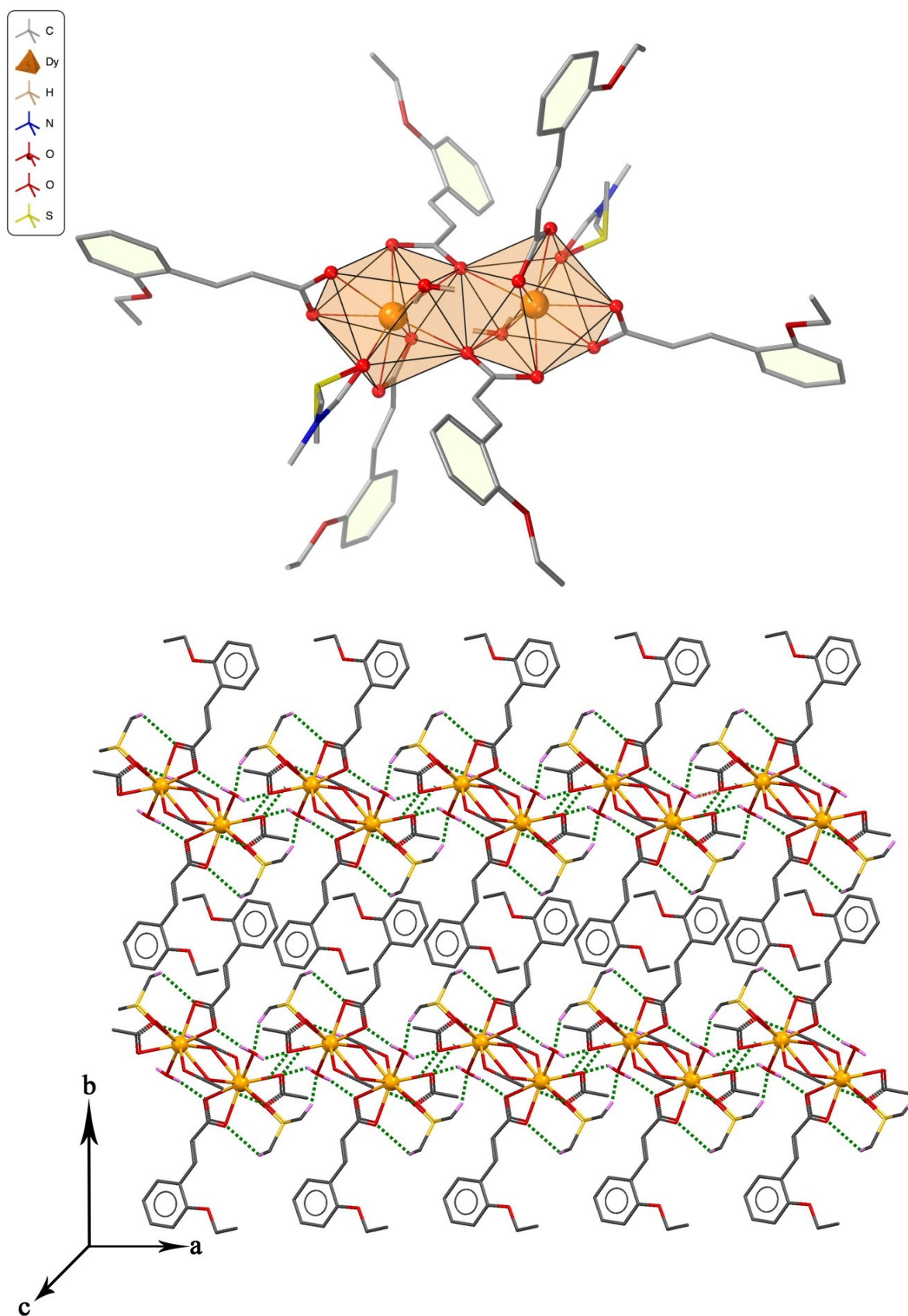
### **Synthesis, structure and magnetic investigations of dinuclear lanthanide complexes based on 2-ethoxycinnamate..**

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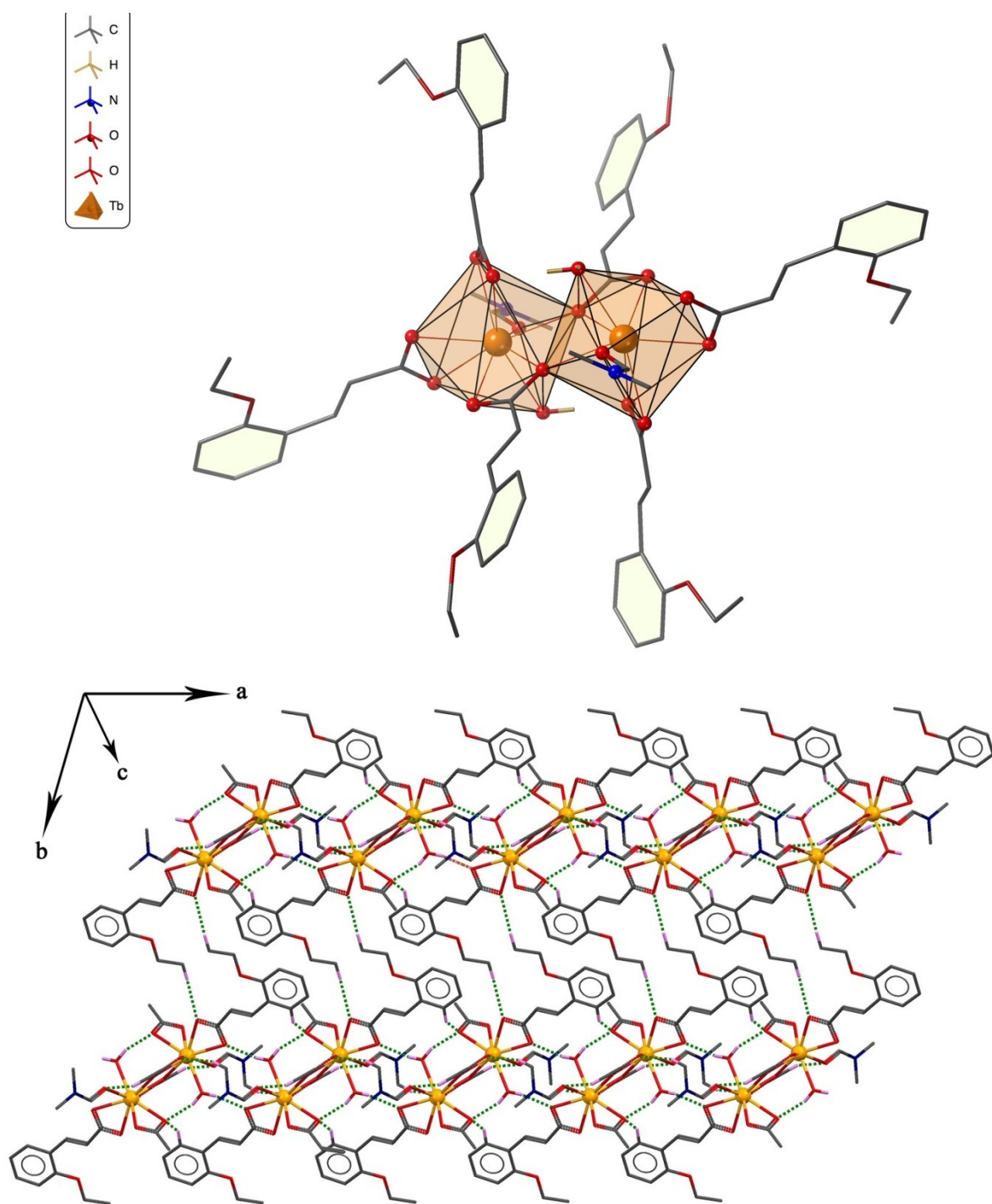
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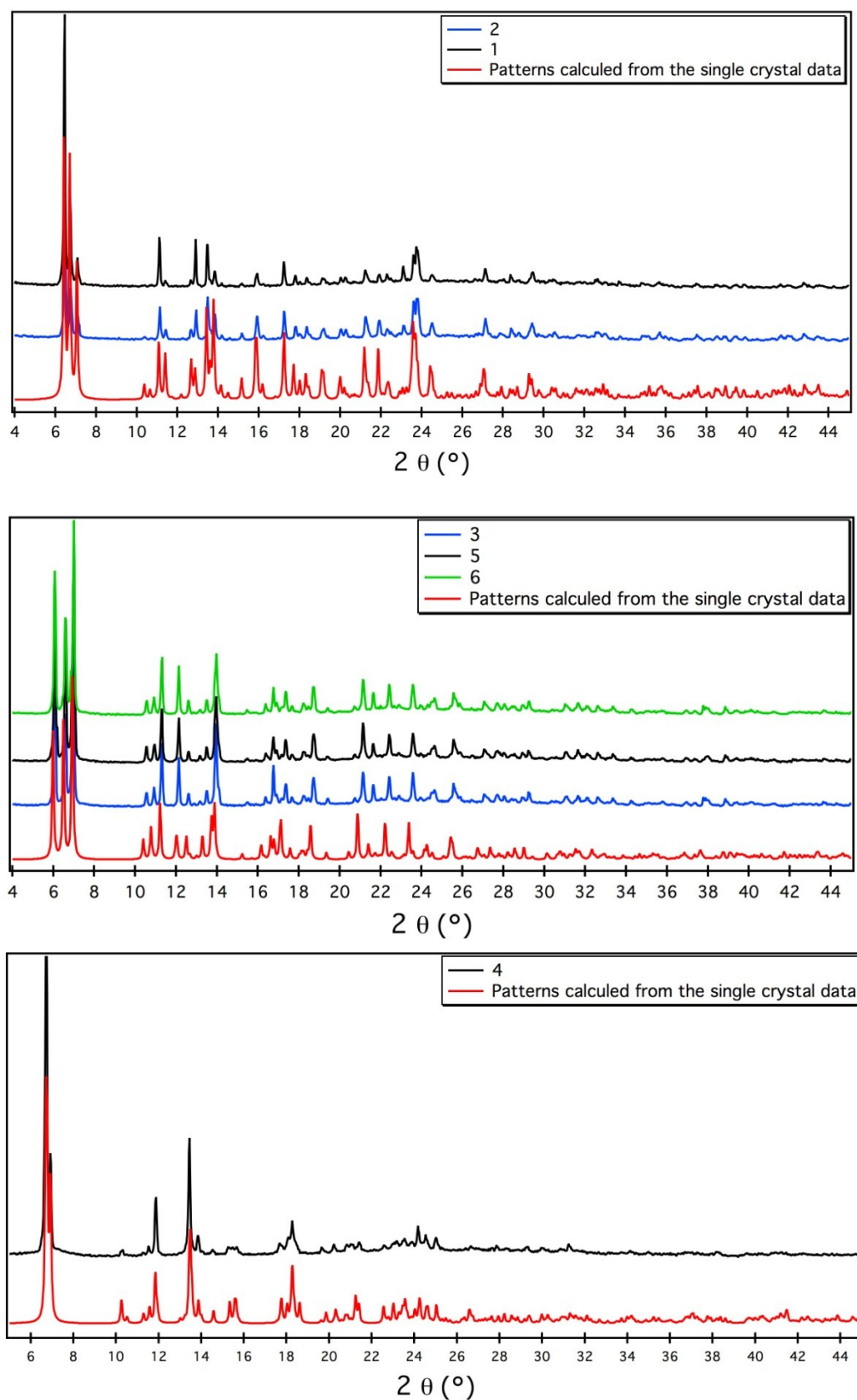
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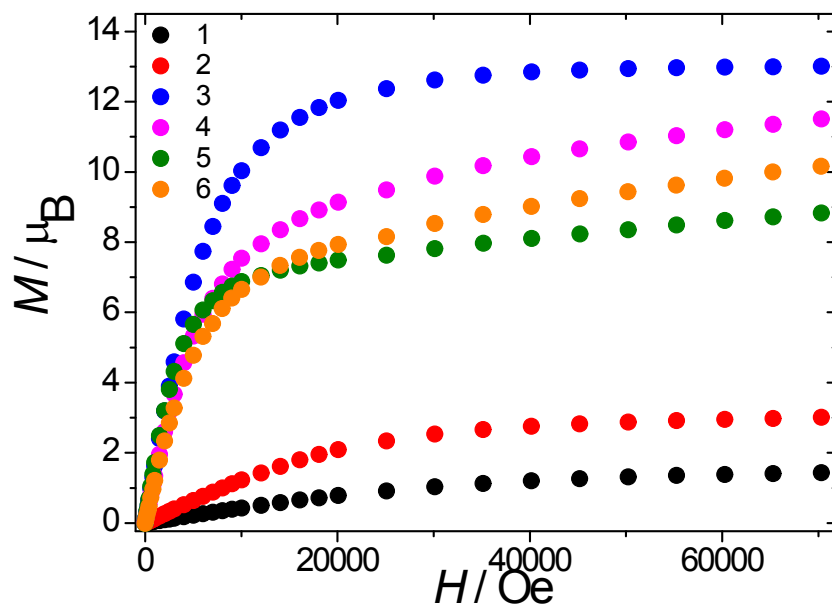
**Figure S1:** Top: Structure of the dinuclear complexes (**3**, **5**, **6**). Hydrogen atoms are omitted for clarity. Bottom: crystal packing.



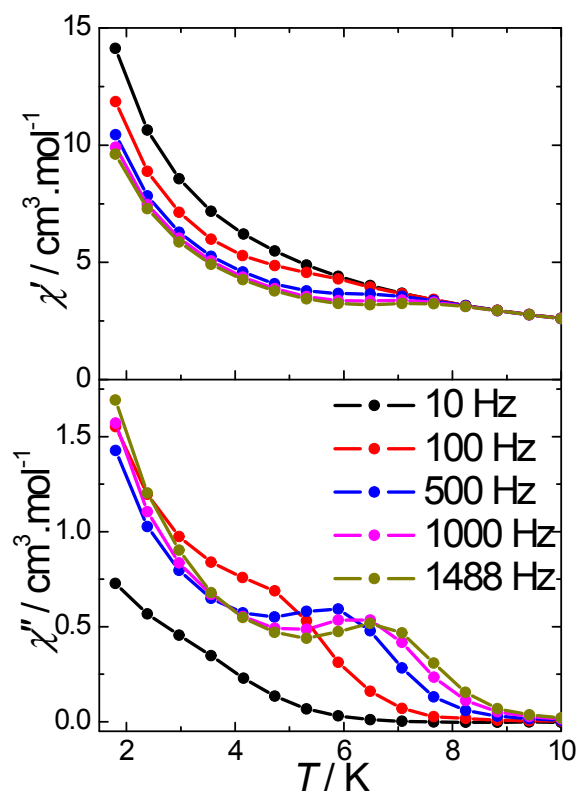
**Figure S2:** Top: Structure of the dinuclear complex **4**. Hydrogen atoms are omitted for clarity.  
Bottom: crystal packing.



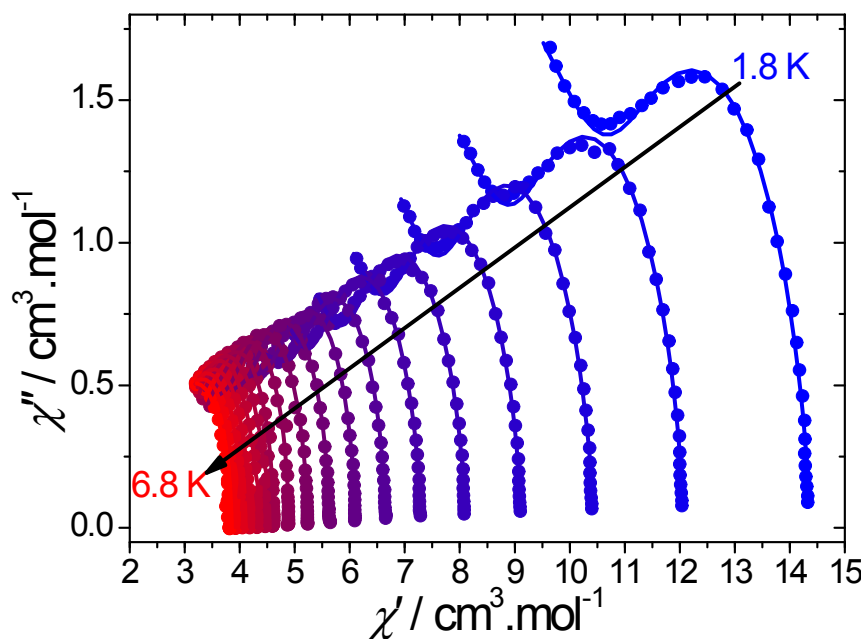
**Figure S3** Powder X-ray diffraction patterns (Cu K $\alpha$ 1) from experiment and simulated for **1-6**.



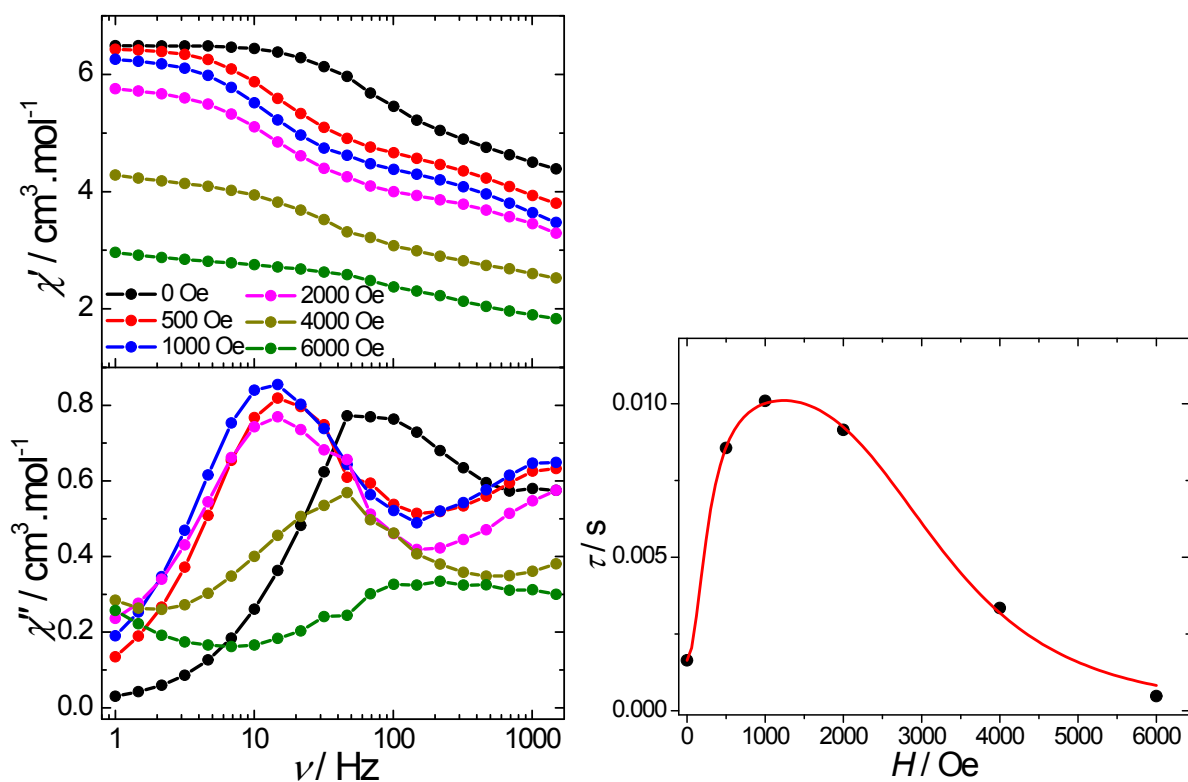
**Figure S4:** Field dependence of the magnetisation at 1.8 K for **1-6**.



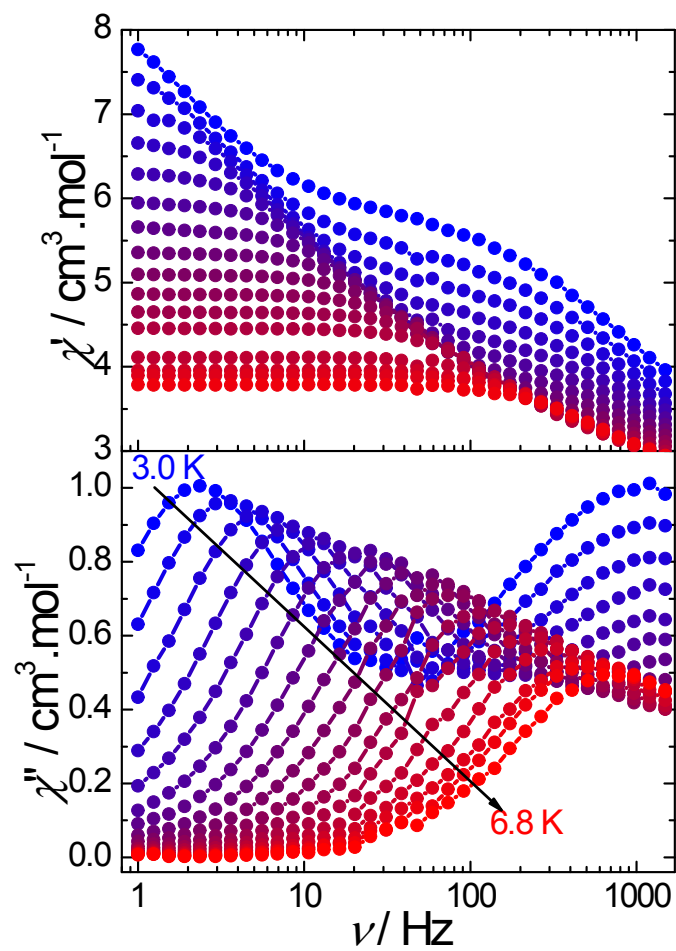
**Figure S5:** Temperature dependence of ac susceptibilities for **5** under a zero dc-field.



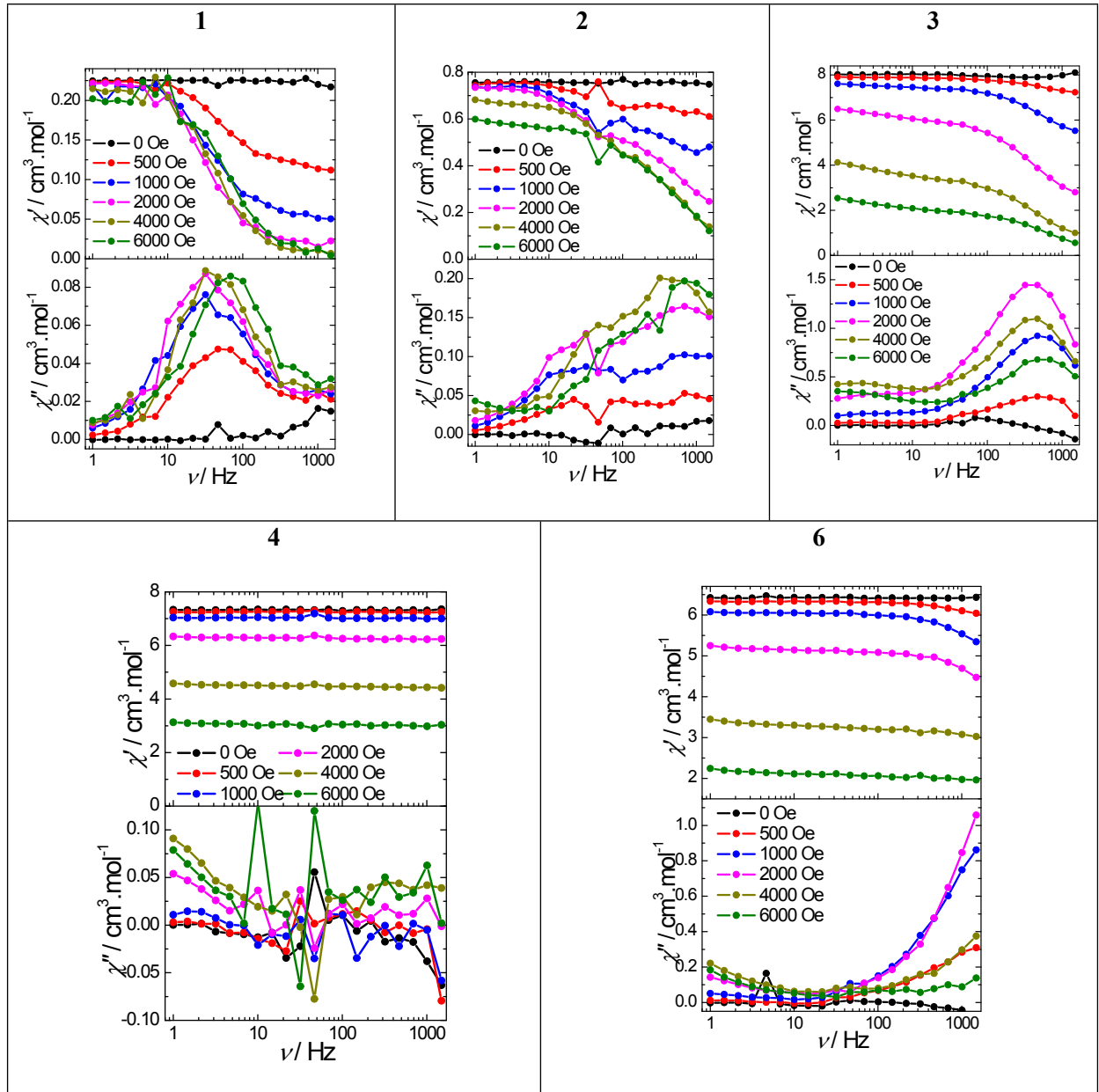
**Figure S6:** Cole-Cole plots using the ac data performed under a zero dc-field for **5**. The solid lines correspond to the fit with a sum of two Debye functions.<sup>1</sup>



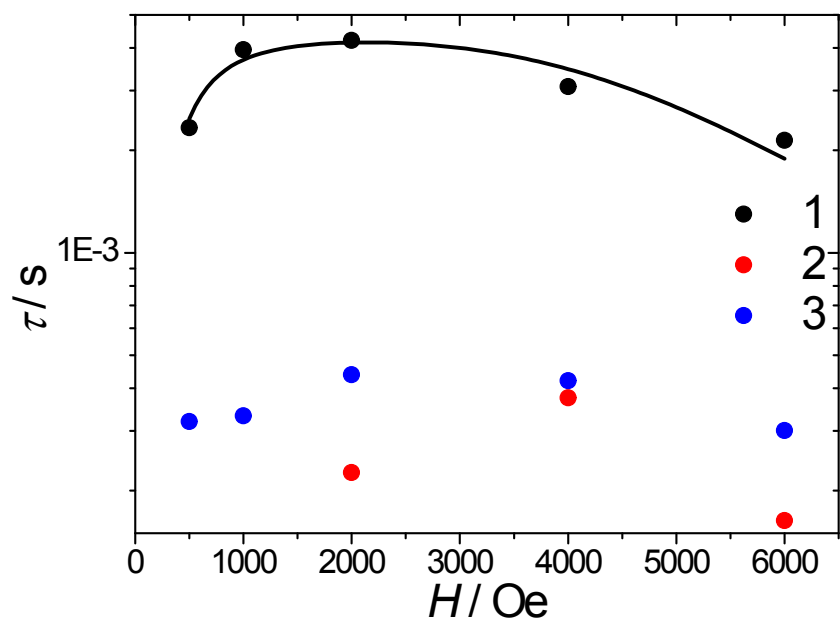
**Figure S7:** Left: frequency dependence of the ac susceptibilities at 4 K for **5** under various dc fields. Right: field dependence of the relaxation time at 4 K for **5**. The red solid line corresponds to the fit with Eq. 2.



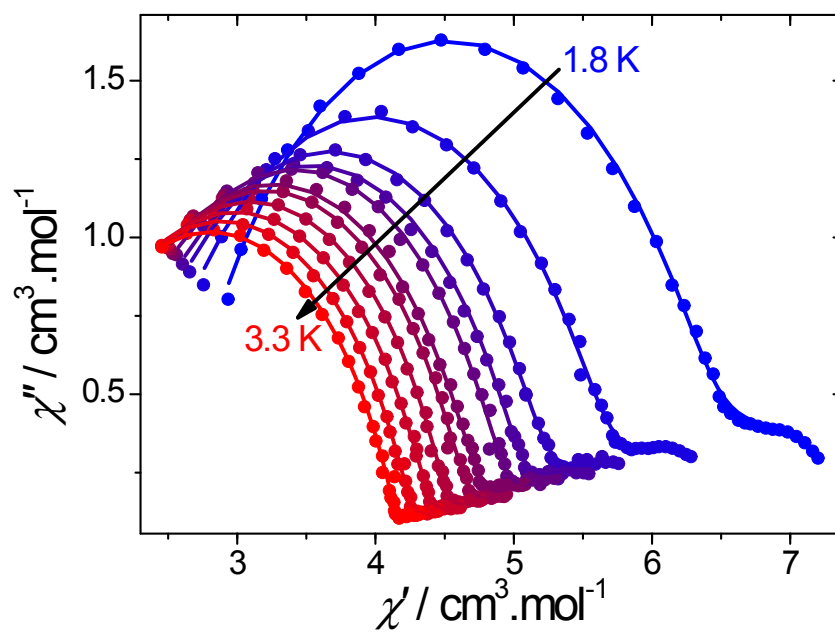
**Figure S8:** Frequency dependence of ac susceptibilities for **5** under a 1000 Oe field.



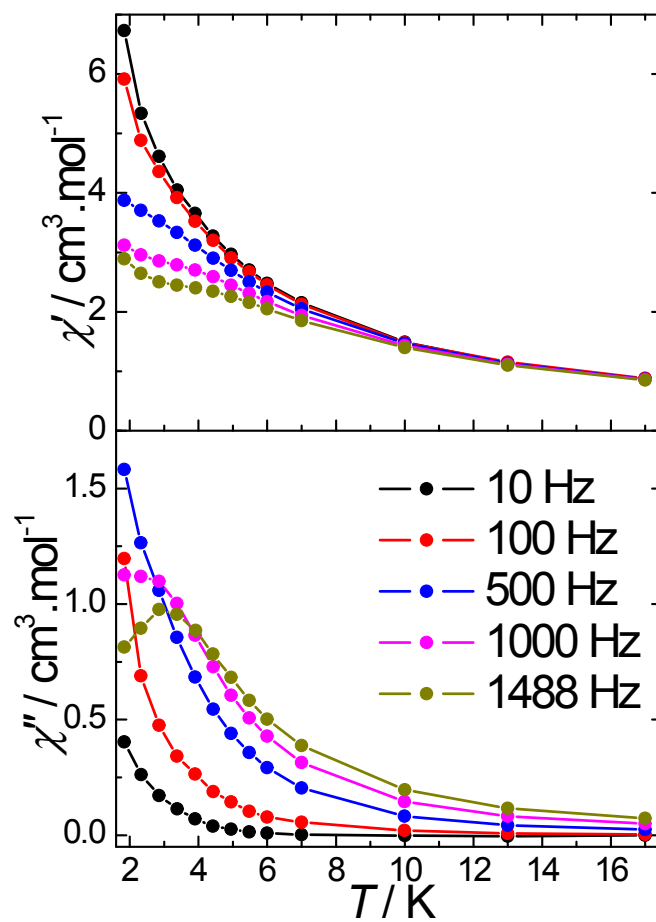
**Figure S9:** Frequency dependence of the ac susceptibilities at 2 K under various dc fields.



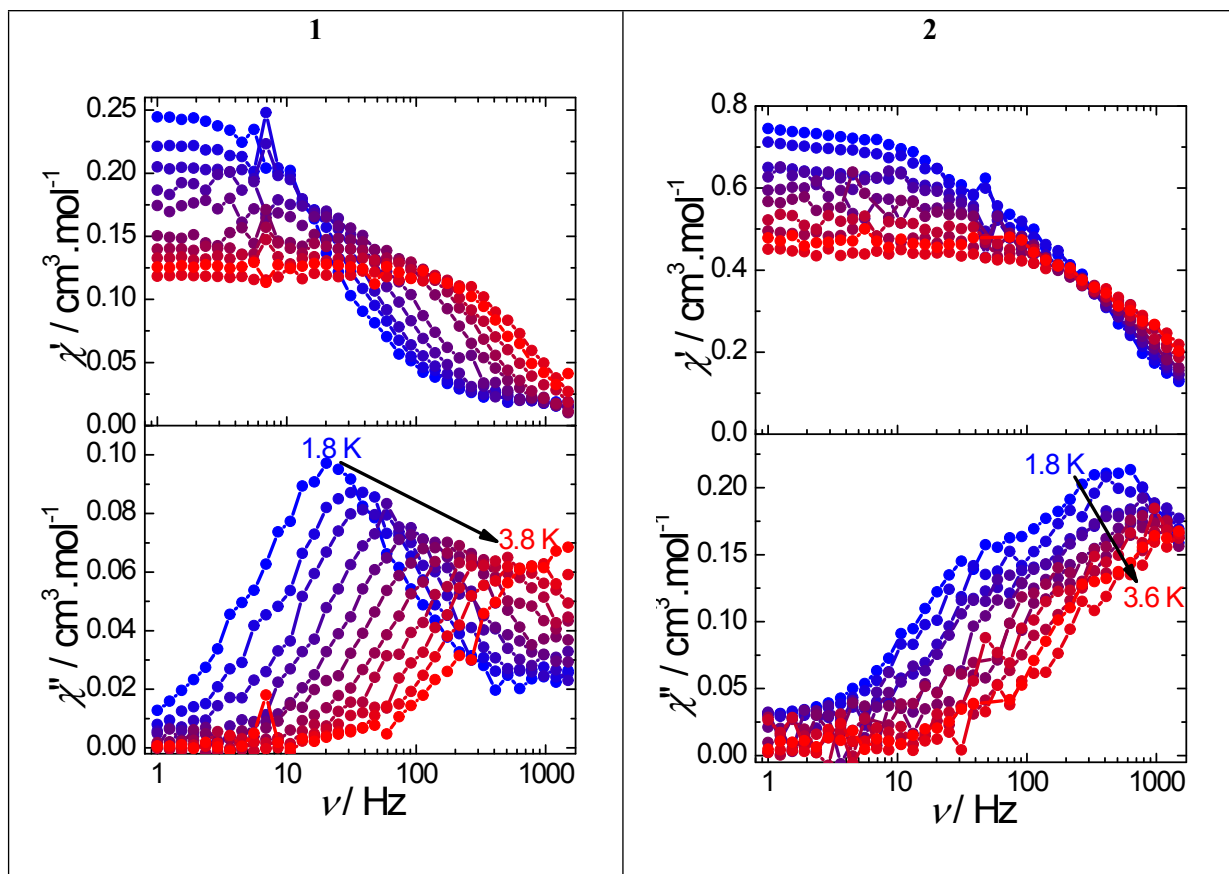
**Figure S10:** Field dependence of the relaxation time at 2 K for **1–3**. The solid line corresponds to the fit with Eq. 2.



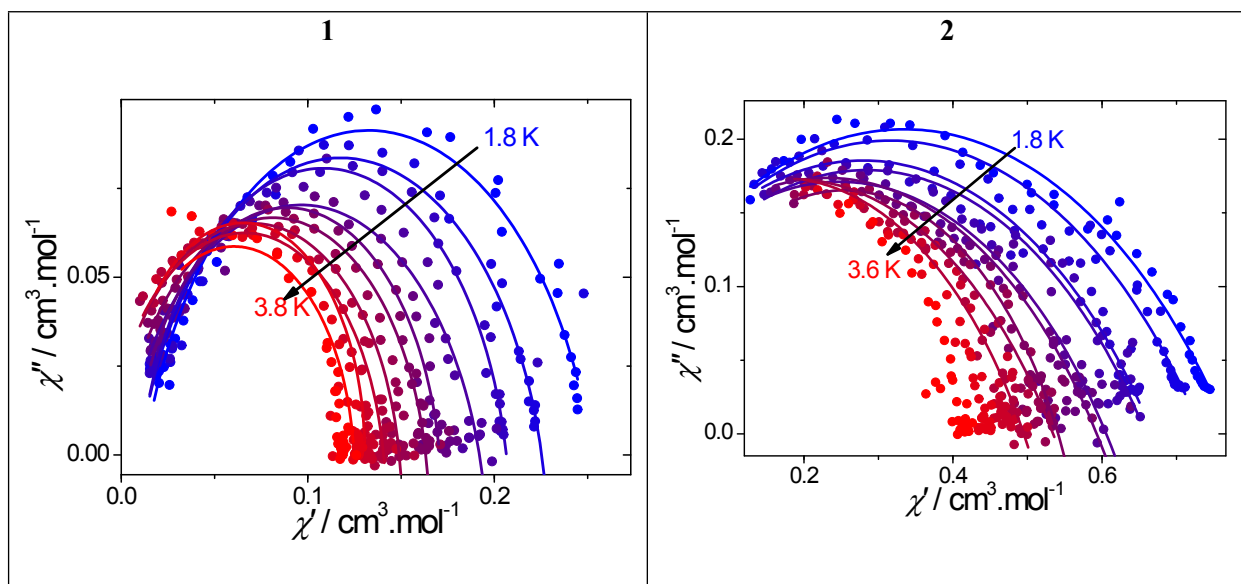
**Figure S11:** Cole-Cole plots using the ac data performed under a 2000 Oe dc-field for **3**. The solid lines correspond to the fit with a sum of two Debye functions.



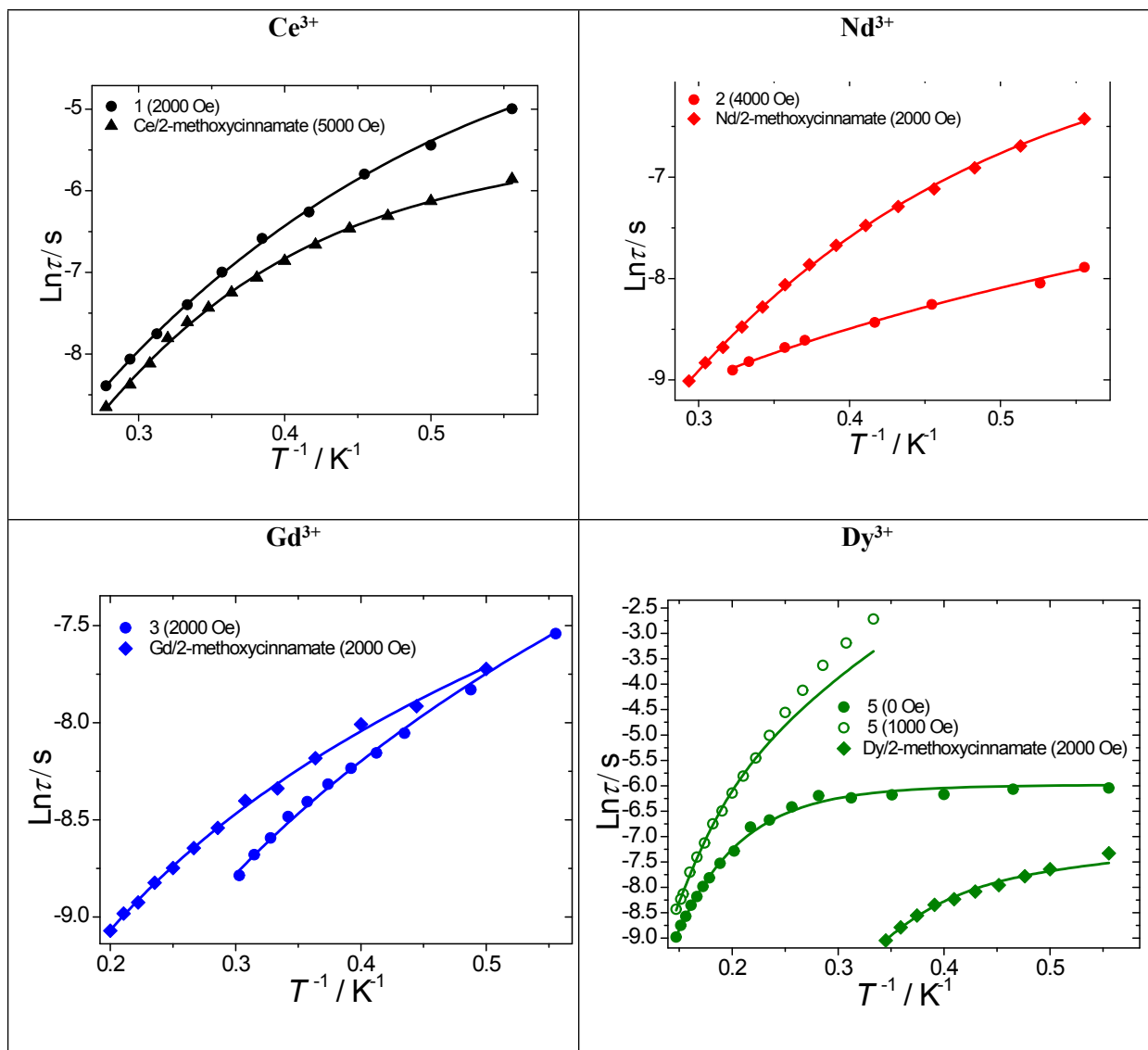
**Figure S12:** Temperature dependence of ac susceptibilities for **3** under a 2000 Oe dc-field.



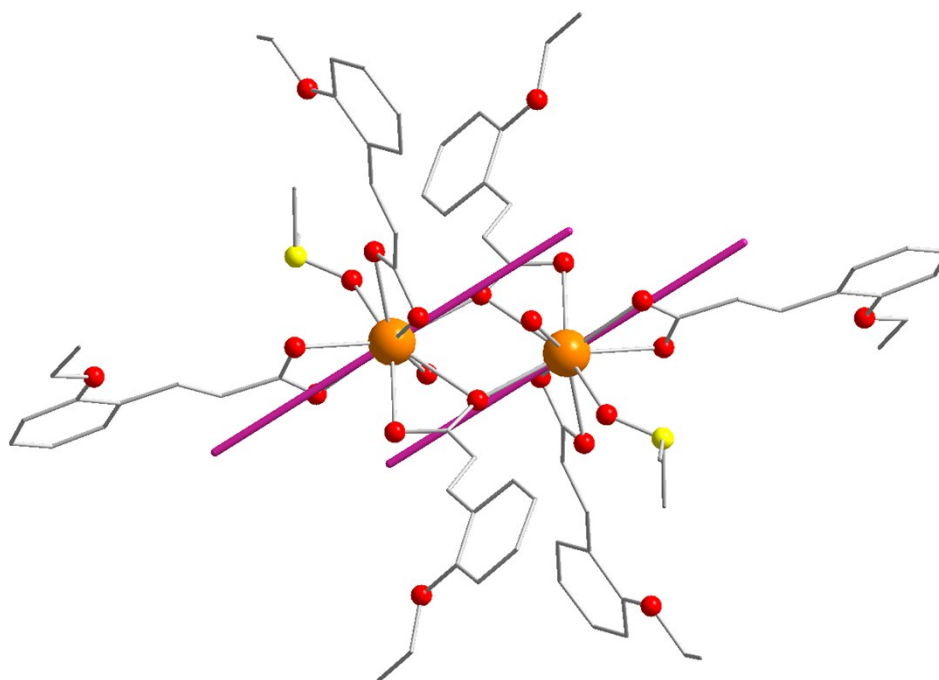
**Figure S13:** Frequency dependence of ac susceptibilities for **1** and **2** under a 2000 Oe and 4000 Oe dc field respectively.



**Figure S14:** Frequency dependence of ac susceptibilities for **1** and **2** under a 2000 Oe and 4000 Oe dc field respectively.



**Figure S15:** Comparison of the temperature dependence of the relaxation time between the dinuclear complexes based on 2-methoxycinnamate ligands.<sup>2</sup>



**Figure S16:** Orientation of the anisotropic axes (purple) in **5**.

**Equation used for the fitting of  $\chi T$  vs.  $T$  for **3**:**

$$\chi_m T = \frac{2N_g^2 \beta^2}{k} \left[ \frac{e^x + 5e^{3x} + 14e^{6x} + 30e^{10x} + 55e^{15x} + 91e^{21x} + 140e^{28x}}{1 + 3e^x + 5e^{3x} + 7e^{6x} + 9e^{10x} + 11e^{15x} + 13e^{21x} + 15e^{28x}} \right]$$

with  $x = J/kT$

**Table S1:** Crystal data and experimental parameters of structures **1 - 6**.

| Complexes reference                                                                      | 1                                                   | 2                                                   | 3                                                                                       | 4                                                  | 5                                                                                       | 6                                                                                       |
|------------------------------------------------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
| <b>Formula</b>                                                                           | C <sub>35</sub> H <sub>41</sub> CeO <sub>11</sub> S | C <sub>35</sub> H <sub>41</sub> NdO <sub>11</sub> S | C <sub>35.4</sub> H <sub>40.3</sub> GdN <sub>0.3</sub> O <sub>11</sub> S <sub>0.7</sub> | C <sub>36</sub> H <sub>42</sub> TbNO <sub>11</sub> | C <sub>35.7</sub> H <sub>41.7</sub> DyN <sub>0.7</sub> O <sub>11</sub> S <sub>0.3</sub> | C <sub>35.6</sub> H <sub>39.8</sub> ErN <sub>0.6</sub> O <sub>11</sub> S <sub>0.4</sub> |
| <b>Mass Mw (g/mol)</b>                                                                   | 809.86                                              | 813.98                                              | 824.17                                                                                  | 823.62                                             | 828..81                                                                                 | 832.16                                                                                  |
| <b>Crystal system</b>                                                                    | Triclinic                                           | Triclinic                                           | Triclinic                                                                               | Triclinic                                          | Triclinic                                                                               | Triclinic                                                                               |
| <b>Space group</b>                                                                       | P-1                                                 | P-1                                                 | P-1                                                                                     | P-1                                                | P-1                                                                                     | P-1                                                                                     |
| <b>Temperature (K)</b>                                                                   | 200                                                 | 300                                                 | 200                                                                                     | 200                                                | 200                                                                                     | 200                                                                                     |
| <b>a (Å)</b>                                                                             | 8.8932(16)                                          | 8.8882(6)                                           | 8.544(7)                                                                                | 9.0353(3)                                          | 8.3946(2)                                                                               | 8.432(5)                                                                                |
| <b>b(Å)</b>                                                                              | 15.015(2)                                           | 15.1063(9)                                          | 14.813(14)                                                                              | 15.2780(6)                                         | 14.6797(4)                                                                              | 14.743(9)                                                                               |
| <b>c(Å)</b>                                                                              | 15.167(2)                                           | 15.1815(9)                                          | 16.466(16)                                                                              | 15.3738(6)                                         | 16.3326(5)                                                                              | 16.443(11)                                                                              |
| <b>α(°)</b>                                                                              | 65.588(11)                                          | 65.367(4)                                           | 110.47(3)                                                                               | 60.453(2)                                          | 110.372(1)                                                                              | 110.89(2)                                                                               |
| <b>γ(°)</b>                                                                              | 87.938(13)                                          | 87.895(4)                                           | 103.78(2)                                                                               | 74.399(2)                                          | 103.423(2)                                                                              | 103.676(16)                                                                             |
| <b>β(°)</b>                                                                              | 74.661(13)                                          | 74.296(4)                                           | 95.51(3)                                                                                | 89.018(2)                                          | 95.963(2)                                                                               | 95.403(14)                                                                              |
| <b>V(Å<sup>3</sup>)</b>                                                                  | 1772.3(5)                                           | 1777.0(2)                                           | 1859(3)                                                                                 | 1761.24(2)                                         | 1797.20(9)                                                                              | 1819.46(2)                                                                              |
| <b>Z</b>                                                                                 | 2                                                   | 2                                                   | 2                                                                                       | 2                                                  | 2                                                                                       | 2                                                                                       |
| <b>dcalc. (g.cm<sup>-1</sup>)</b>                                                        | 1.518                                               | 1.521                                               | 1.472                                                                                   | 1.553                                              | 1.532                                                                                   | 1.519                                                                                   |
| <b>μ (mm<sup>-1</sup>)</b>                                                               | 10.97                                               | 12.19                                               | 12.35                                                                                   | 10.39                                              | 11.80                                                                                   | 4.99                                                                                    |
| <b>R<sub>i</sub>[I &gt; 2σ(I)]</b>                                                       | 0.067                                               | 0.041                                               | 0.050                                                                                   | 0.033                                              | 0.033                                                                                   | 0.044                                                                                   |
| <b>wR<sub>i</sub>[I &gt; 2σ(I)]</b>                                                      | 0.158                                               | 0.142                                               | 0.128                                                                                   | 0.097                                              | 0.105                                                                                   | 0.123                                                                                   |
| <b>GOF (F<sup>2</sup>)</b>                                                               | 0.99                                                | 1.09                                                | 0.993                                                                                   | 1.095                                              | 1.047                                                                                   | 1.024                                                                                   |
| <b>Residual electron density, e Å<sup>-3</sup><br/>(ρ<sub>min</sub>/ρ<sub>max</sub>)</b> | 1.21/-1.35                                          | 0.91/-1.02                                          | 1.12/-1.03                                                                              | 0.85/-0.75                                         | 0.56/-0.74                                                                              | 1.00/-0.94                                                                              |

$$^a R1 = \sum ||F_o| - |F_c|| / \sum |F_o|; ^b wR2 = \sqrt{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]}$$

**Table S2.** Selected bond distances (Å) and bond angles (°).

|                                   | 1          | 2         | 3           | 4           | 5           | 6           |
|-----------------------------------|------------|-----------|-------------|-------------|-------------|-------------|
| <b>Ln—O1</b>                      | 2.492 (8)  | 2.478 (6) | 2.497 (5)   | 2.393 (3)   | 2.457 (3)   | 2.439 (4)   |
| <b>Ln—O1W</b>                     | 2.557 (9)  | 2.528 (6) | 2.397 (5)   | 2.428 (3)   | 2.353 (3)   | 2.336 (4)   |
| <b>Ln—O2</b>                      | 2.531 (3)  | 2.515 (6) | 2.426 (5)   | 2.478 (3)   | 2.391 (3)   | 2.396 (4)   |
| <b>Ln—O4</b>                      | 2.519 (8)  | 2.473 (7) | 2.471 (5)   | 2.448 (3)   | 2.446 (3)   | 2.434 (4)   |
| <b>Ln—O5</b>                      | 2.540 (9)  | 2.510 (7) | 2.454 (5)   | 2.442 (3)   | 2.413 (3)   | 2.404 (4)   |
| <b>Ln—O7<sup>i</sup></b>          | 2.562 (8)  | 2.518 (7) | 2.501 (5)   | 2.483 (3)   | 2.459 (3)   | 2.451 (4)   |
| <b>Ln—O8</b>                      | 2.464 (9)  | 2.434 (6) | 2.468 (5)   | 2.400 (3)   | 2.405 (3)   | 2.388 (4)   |
| <b>Ln—O8<sup>i</sup></b>          | 2.710 (9)  | 2.680 (7) | 2.563 (5)   | 2.499 (2)   | 2.529 (3)   | 2.541 (4)   |
| <b>Ln—O10</b>                     | 2.470 (10) | 2.445 (7) | 2.410 (5)   | 2.384 (3)   | 2.380 (3)   | 2.363 (4)   |
| <b>O1—Ln—<br/>O1W</b>             | 158.8 (3)  | 157.6 (2) | 128.00 (16) | 127.02 (10) | 128.15 (10) | 128.53 (13) |
| <b>O1—Ln—O4</b>                   | 77.4 (3)   | 76.7 (2)  | 74.36 (18)  | 74.50 (11)  | 74.42 (11)  | 74.22 (15)  |
| <b>O1—Ln—O5</b>                   | 102.0 (3)  | 102.8 (2) | 86.06 (16)  | 79.01 (10)  | 86.00 (10)  | 84.81 (14)  |
| <b>O1—Ln—O7<sup>i</sup></b>       | 76.3 (3)   | 76.0 (3)  | 78.95 (19)  | 71.70 (11)  | 79.10 (11)  | 78.80 (15)  |
| <b>O1—Ln—O8<sup>i</sup></b>       | 107.7 (3)  | 108.1 (2) | 129.11 (17) | 113.68 (10) | 130.14 (10) | 129.83 (15) |
| <b>O1W—Ln—<br/>O7<sup>i</sup></b> | 90.5 (3)   | 89.2 (2)  | 97.2 (2)    | 78.02 (10)  | 97.47 (11)  | 96.32 (15)  |
| <b>O1W—Ln—<br/>O8<sup>i</sup></b> | 74.1 (3)   | 72.9 (2)  | 74.96 (17)  | 75.71 (9)   | 74.49 (10)  | 74.18 (13)  |
| <b>O4—Ln—O7<sup>i</sup></b>       | 153.6 (3)  | 152.6 (3) | 122.82 (18) | 136.41 (11) | 123.29 (11) | 123.93 (14) |
| <b>O4—Ln—<br/>O1W</b>             | 115.4 (3)  | 117.6 (2) | 138.73 (19) | 145.47 (10) | 138.02 (11) | 138.60 (15) |
| <b>O4—Ln—O8<sup>i</sup></b>       | 140.1 (3)  | 139.9 (2) | 121.18 (17) | 124.08 (9)  | 121.07 (10) | 120.93 (12) |
| <b>O5—Ln—O8<sup>i</sup></b>       | 149.9 (3)  | 148.9 (2) | 73.51 (16)  | 73.27 (9)   | 73.30 (10)  | 73.35 (12)  |
| <b>O5—Ln—O7<sup>i</sup></b>       | 138.2 (3)  | 138.8 (2) | 75.69 (17)  | 93.32 (10)  | 75.28 (10)  | 75.47 (13)  |
| <b>O8—Ln—O1</b>                   | 125.5 (3)  | 126.8 (2) | 153.10 (17) | 152.20 (10) | 152.55 (11) | 152.05 (13) |
| <b>O8—Ln—O7<sup>i</sup></b>       | 114.5 (3)  | 114.5 (2) | 115.25 (16) | 115.88 (9)  | 115.81 (10) | 116.06 (13) |
| <b>O8—Ln—O10</b>                  | 153.7 (3)  | 152.6 (3) | 88.71 (18)  | 78.52 (9)   | 89.28 (10)  | 89.25 (14)  |
| <b>O10—Ln—O2</b>                  | 128.86 (3) | 129.4 (2) | 75.87 (18)  | 74.49 (10)  | 75.22 (11)  | 75.03 (14)  |
| <b>O10—Ln—O8<sup>i</sup></b>      | 112.4 (3)  | 113.1 (2) | 144.24 (17) | 134.48 (10) | 144.26 (10) | 144.08 (14) |

Symmetry transformations used to generate equivalent atoms: Symmetry code: (i) -x, 1-y, 1-z.

**Table S3.** SHAPE analysis.

|          | JJCU   | CCU   | JCSAPR | CSAPR | JTCTPR | TCTPR |
|----------|--------|-------|--------|-------|--------|-------|
| <b>1</b> | 8.035  | 7.093 | 4.739  | 4.115 | 6.213  | 4.834 |
| <b>2</b> | 8.130  | 7.237 | 4.345  | 3.743 | 5.952  | 4.536 |
| <b>3</b> | 10.065 | 8.586 | 3.192  | 2.070 | 3.675  | 2.784 |
| <b>4</b> | 9.835  | 8.009 | 3.258  | 2.453 | 4.631  | 2.702 |
| <b>5</b> | 9.935  | 8.504 | 2.998  | 1.91  | 3.476  | 2.667 |
| <b>6</b> | 9.888  | 8.849 | 2.929  | 1.871 | 3.258  | 2.514 |

JJCU: Capped cube  
CCU: Spherical-relaxed capped cube  
JCSAPR: Capped square antiprism  
CSAPR: Spherical capped square antiprism  
JTCTPR: Tricapped trigonal prism  
TCTPR: Spherical tricapped trigonal prism

**Table S4.** Fitting of the Cole-Cole plots with a sum of two generalized Debye functions for temperature ranging from 1.8 to 6.9 K under a zero dc-field for **5**.

| <b><i>T</i> (K)</b> | <b><math>\chi_{S_{tot}}</math></b> | <b><math>\Delta\chi_1</math></b> | <b><math>\alpha_1</math></b> | <b><math>\Delta\chi_2</math></b> | <b><math>\alpha_2</math></b> |
|---------------------|------------------------------------|----------------------------------|------------------------------|----------------------------------|------------------------------|
| 1.8                 | 3.30295                            | 3.30955                          | 0.1491                       | 7.78267                          | 0.37153                      |
| 2.15                | 2.86004                            | 2.83325                          | 0.141                        | 6.4032                           | 0.37573                      |
| 2.5                 | 0.78189                            | 2.44918                          | 0.13354                      | 7.22443                          | 0.42422                      |
| 2.85                | 1.28579                            | 2.20849                          | 0.13831                      | 5.65515                          | 0.41518                      |
| 3.2                 | 1.73312                            | 1.9988                           | 0.12935                      | 4.39413                          | 0.39736                      |
| 3.55                | 1.85616                            | 1.79398                          | 0.10921                      | 3.66252                          | 0.39526                      |
| 3.9                 | 3.06094                            | 1.43072                          | 0.05957                      | 2.17944                          | 0.38316                      |
| 4.25                | 3.22171                            | 1.36357                          | 0.05171                      | 1.52867                          | 0.31532                      |
| 4.6                 | 3.06674                            | 1.3275                           | 0.05683                      | 1.24661                          | 0.28313                      |
| 4.95                | 2.88628                            | 1.28749                          | 0.05687                      | 1.06648                          | 0.24005                      |
| 5.3                 | 3.03102                            | 1.01216                          | 1.59134E-15                  | 0.84772                          | 0.1686                       |
| 5.6                 | 2.95678                            | 0.92681                          | 3.18795E-15                  | 0.73082                          | 0.08695                      |
| 5.8                 | 2.83884                            | 0.90866                          | 2.3744E-15                   | 0.72276                          | 0.08666                      |
| 6                   | 2.73468                            | 0.80805                          | 2.90533E-15                  | 0.77797                          | 0.10866                      |
| 6.2                 | 2.67117                            | 0.68537                          | 4.00678E-15                  | 0.82474                          | 0.13549                      |

|     |         |         |             |         |         |
|-----|---------|---------|-------------|---------|---------|
| 6.4 | 2.4146  | 0.6587  | 7.45678E-15 | 0.98125 | 0.23567 |
| 6.6 | 2.29506 | 0.67641 | 8.18393E-15 | 0.95767 | 0.20202 |
| 6.8 | 3.30295 | 3.30955 | 1.03612E-14 | 0.94686 | 0.17624 |

**Table S5.** Fit parameters of the field dependence of the relaxation time obtained using the Eq. 1

| <i>Compound</i> | <i>D (s<sup>-1</sup>K<sup>-1</sup>Oe<sup>-4</sup>)</i> | <i>B<sub>1</sub> (s<sup>-1</sup>)</i> | <i>B<sub>2</sub> (Oe<sup>-2</sup>)</i> | <i>K</i> |
|-----------------|--------------------------------------------------------|---------------------------------------|----------------------------------------|----------|
| <b>1</b> (2 K)  | $1.16 \times 10^{-1}$                                  | 93218                                 | $2.09 \times 10^{-3}$                  | 226.22   |
| <b>5</b> (4 K)  | $2.15 \times 10^{-13}$                                 | 517.14                                | $8.38 \times 10^{-5}$                  | 93.9     |

**Table S6.** Fitting of the Cole-Cole plots with a sum of two generalized Debye functions under a 2000 Oe dc-field for **3**.

| <i>T (K)</i> | <i>χ<sub>S tot.</sub></i> | <i>Δχ<sub>1</sub></i> | <i>α<sub>1</sub></i> | <i>Δχ<sub>2</sub></i> | <i>α<sub>2</sub></i> |
|--------------|---------------------------|-----------------------|----------------------|-----------------------|----------------------|
| 1.8          | 2.55093                   | 3.77723               | 0.11529              | 1.25618               | 0.39325              |
| 2.05         | 2.24909                   | 3.29527               | 0.13154              | 1.36141               | 0.4797               |
| 2.3          | 2.0956                    | 3.01963               | 0.12599              | 1.30041               | 0.50123              |
| 2.425        | 1.99453                   | 3.00598               | 0.13756              | 0.94658               | 0.41612              |
| 2.55         | 1.89493                   | 2.93523               | 0.13342              | 1.34498               | 0.55692              |
| 2.675        | 1.77064                   | 2.87291               | 0.14387              | 1.31956               | 0.5774               |
| 2.8          | 1.74971                   | 2.77603               | 0.13582              | 1.28772               | 0.63695              |
| 2.925        | 1.67364                   | 2.80492               | 0.15187              | 0.74517               | 0.48673              |
| 3.05         | 1.58307                   | 2.74504               | 0.15917              | 0.78248               | 0.56273              |
| 3.175        | 1.52651                   | 2.68258               | 0.16                 | 0.75889               | 0.56098              |
| 3.3          | 1.45664                   | 2.69224               | 0.17718              | 0.35393               | 0.31858              |

**Table S7.** Fitting of the Cole-Cole plots with a generalized Debye model under a 2000 Oe dc-field for **1**.

| <i>T (K)</i> | <i>α</i> | <i>χ<sub>S</sub> (cm<sup>3</sup>. mol<sup>-1</sup>)</i> | <i>χ<sub>T</sub> (cm<sup>3</sup>. mol<sup>-1</sup>)</i> |
|--------------|----------|---------------------------------------------------------|---------------------------------------------------------|
|--------------|----------|---------------------------------------------------------|---------------------------------------------------------|

|     |             |         |           |
|-----|-------------|---------|-----------|
| 1.8 | 0.03361     | 0.23124 | 0.20856   |
| 2   | 0.02733     | 0.20766 | 0.19079   |
| 2.2 | 0.02253     | 0.19426 | 0.14107   |
| 2.4 | 0.02013     | 0.17298 | 0.23549   |
| 2.6 | 0.0156      | 0.16232 | 0.11335   |
| 2.8 | 0.01021     | 0.15264 | 0.1477    |
| 3   | 0.00216     | 0.14024 | 0.12795   |
| 3.2 | 2.68102E-15 | 0.13235 | 0.12503   |
| 3.4 | 2E-16       | 0.13061 | 5.3424E-4 |
| 3.6 | 9.53704E-17 | 0.12108 | 0.06149   |

**Table S8.** Fitting of the Cole-Cole plots with a generalized Debye model under a 4000 Oe dc-field for **2**.

| <i>T</i> (K) | $\alpha$ | $\chi_s$ (cm <sup>3</sup> . mol <sup>-1</sup> ) | $\chi_r$ (cm <sup>3</sup> . mol <sup>-1</sup> ) |
|--------------|----------|-------------------------------------------------|-------------------------------------------------|
| 1.8          | 0.29702  | 0.37115                                         | 0.93446                                         |
| 1.9          | 0.26423  | 0.36816                                         | 0.90388                                         |
| 2.1          | 0.22381  | 0.33427                                         | 0.88996                                         |
| 2.2          | 0.2294   | 0.33786                                         | 0.88795                                         |
| 2.4          | 0.18996  | 0.30506                                         | 0.87506                                         |
| 2.5          | 0.16519  | 0.29595                                         | 0.85939                                         |
| 2.7          | 0.08931  | 0.4191                                          | 0.50301                                         |
| 2.8          | 0.07941  | 0.29146                                         | 0.75831                                         |
| 3            | 0.01865  | 0.32063                                         | 0.61464                                         |

**Table S9.** SHAPE analysis comparison between the dysprosium dinuclear complex based on 2-ethoxycinnamate and 2-methoxycinnamate.

| JJCU | CCU | JCSAPR | CSAPR | JTCTPR | TCTPR |
|------|-----|--------|-------|--------|-------|
|------|-----|--------|-------|--------|-------|

|                                           |        |       |       |       |       |       |
|-------------------------------------------|--------|-------|-------|-------|-------|-------|
| <b>5 (2 ethoxycinnamate)</b>              | 9.935  | 8.504 | 2.998 | 1.91  | 3.476 | 2.667 |
| <b>Dy (2-methoxycinnamate)</b>            | 10.193 | 8.797 | 3.103 | 2.296 | 3.407 | 3.058 |
| JJCUCapped cube                           |        |       |       |       |       |       |
| CCU: Spherical-relaxed capped cube        |        |       |       |       |       |       |
| JCSAPR: Capped square antiprism           |        |       |       |       |       |       |
| CSAPR: Spherical capped square antiprism  |        |       |       |       |       |       |
| JTCTPR: Tricapped trigonal prism          |        |       |       |       |       |       |
| TCTPR: Spherical tricapped trigonal prism |        |       |       |       |       |       |

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