Supplementary Material (ESI) for Dalton Transactions


# Electronic Supplementary Information

# Two $Mn^{II}_2Ln^{III}_4$ (Ln = Gd, Eu) hexanuclear compounds of *p-tert*-butylsulfinylcalix[4]arene

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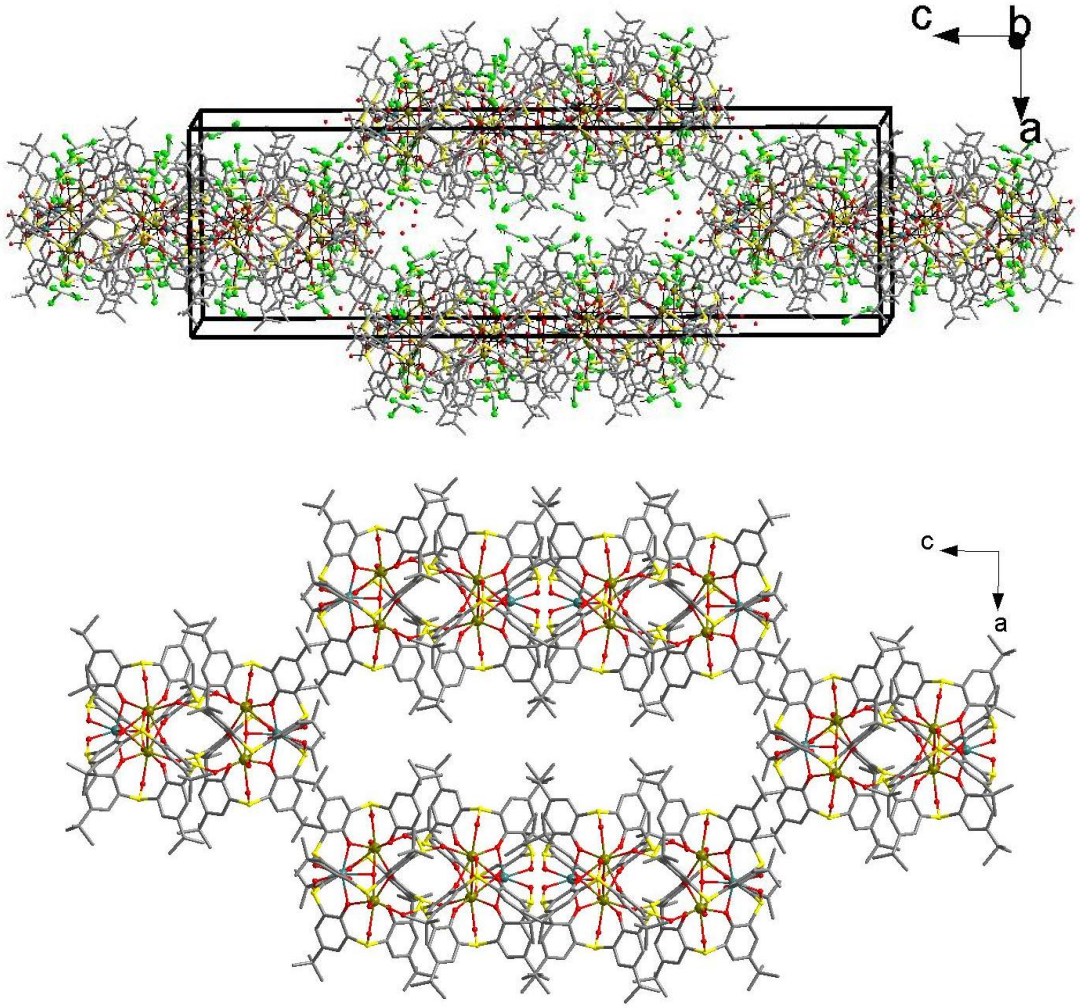


**Fig. S1** Views of the extended structure of **1** with (upper) and without the solvent molecules (bottom).

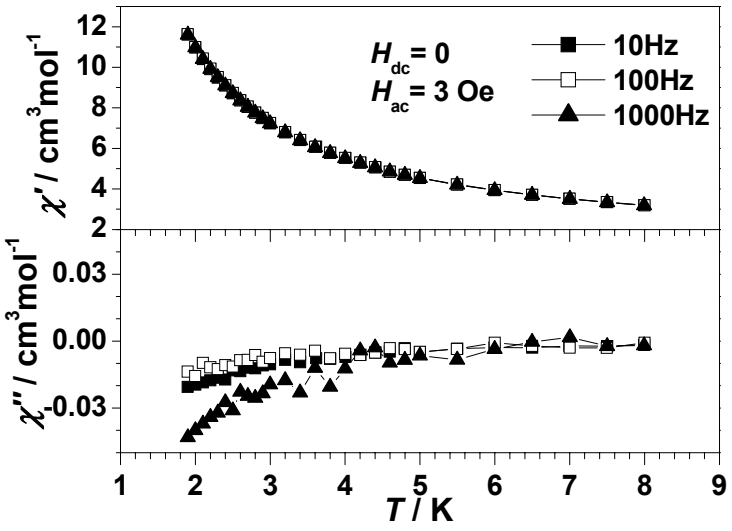


**Fig. S2** ac susceptibility measurement for **1**

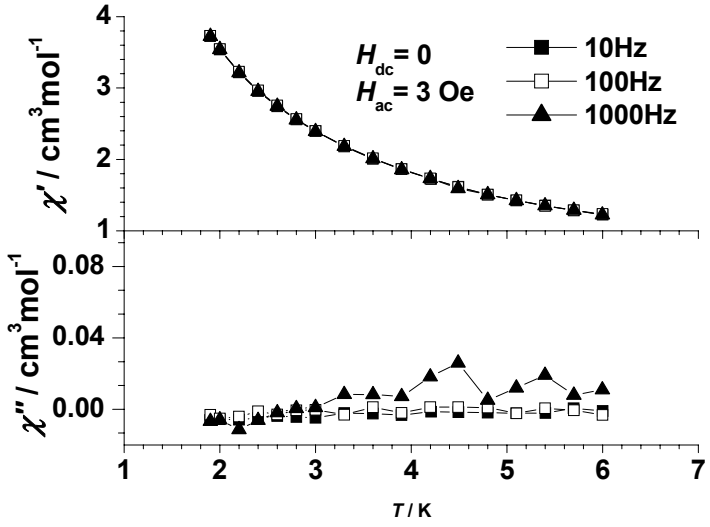


**Fig. S3** ac susceptibility measurement for **2**

**Table S1**. Selected bond distances (Å) and angles (º) for compounds **1** and **2** (based on squeezed data)

| **1** | | **2** | |
|---|---|---|---|
| Gd(1)–O(1) | 2.454(2) | Eu(1)–O(1) | 2.461(2) |
| Gd(1)–O(2) | 2.317(2) | Eu (1)–O(2) | 2.326(2) |
| Gd(1)–O(3) | 2.348(2) | Eu (1)–O(3) | 2.362(2) |
| Gd(1)–O(4) | 2.402(2) | Eu (1)–O(4) | 2.407(2) |
| Gd(1)–O(6) | 2.351(2) | Eu (1)–O(6) | 2.361(2) |
| Gd(1)–O(7) | 2.388(2) | Eu (1)–O(7) | 2.393(2) |
| Gd(1)–O(8) | 2.343(2) | Eu (1)–O(8) | 2.354(2) |
| Gd(1)–O(9) | 2.3682(2) | Eu (1)–O(9) | 2.3767(2) |
| | | | |
| Mn(1)–O(1) | 2.210(2) | Mn(1)–O(1) | 2.208(2) |
| Mn(1)–O(4) | 2.219(2) | Mn(1)–O(4) | 2.215(2) |
| Mn(1)–O(5) | 2.096(5) | Mn(1)–O(5) | 2.109(5) |
| Mn(1)–O(9) | 2.234(3) | Mn(1)–O(9) | 2.227(3) |
| | | | |
| Gd(1)–Mn(1) | 3.3120(5) | Eu(1)–Mn(1) | 3.3130(5) |
| Gd(1)–Gd(1) | 4.7336(2) | Eu(1)–Eu(1) | 4.7506(3) |
| | | | |
| Mn(1)–O(1)–Gd(1) | 90.32(7) | Mn(1)–O(1)–Eu(1) | 90.22(7) |
| Mn(1)–O(4)–Gd(1) | 91.47(7) | Mn(1)–O(4)–Eu(1) | 91.47(7) |
| Mn(1)–O(9)–Gd(1) | 92.00(7) | Mn(1)–O(9)–Eu(1) | 91.98(7) |
| Gd(1)–O(9)–Gd(1) | 175.99(14) | Eu(1)–O(9)–Eu(1) | 176.03(13) |
| | | | |
| Mn(1)–Gd(1)–Gd(1) | 44.389(2) | Mn(1)–Eu(1)–Eu(1) | 44.195(3) |
| Gd(1)–Mn(1)–Gd(1) | 91.220(16) | Eu(1)–Mn(1)–Eu(1) | 91.610(16) |

**Table S2** Crystallographic data for compounds **1** and **2 (**non-squeezed**)**

| | **1** | **2** |
|---|---|---|
| CCDC- number | 683027 | 683028 |
| Formula | $C_{167.72}H_{200.28}C_{l23.16}Gd_4Mn_2O_{40.28}S_{16}$ | $C_{167.55}H_{198.19}Cl_{22.65}Eu_4Mn_2O_{39.35}S_{16}$ |
| Formula wt. | 4933.50 | 4875.35 |
| Crystal system | Tetragonal | Tetragonal |
| Space group | $I4_1/a$ | $I4_1/a$ |
| $T$ /K | 185(2) | 150(2) |
| $a$ /Å | 19.7575(6) | 19.6997(8) |
| $b$ /Å | 19.7575(6) | 19.6997(8) |
| $c$ /Å | 65.511(3) | 65.255(4) |
| $V$ ( Å $^3$) | 25572.8(16) | 25324(2) |
| $Z$ | 4 | 4 |
| $D_c$/g cm$^{-3}$ | 1.281 | 1.279 |
| $\mu$/mm$^{-1}$ | 1.546 | 1.498 |
| $F$(000) | 9938 | 7864 |
| Tot. Data | 124362 | 256781 |
| Uniq. Data | 14640 | 15242 |
| $\theta_{max}$ | 27.49 | 28.00 |
| $R_{int}$ | 0.028 | 0.055 |
| $GOF$ | 1.06 | 1.028 |
| $R_1$[a] [$I$>2σ($I$)] | 0.0852 | 0.0882 |
| $wR_2$[b](all data) | 0.2676 | 0.2913 |

[a] $R_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$; [b] $wR_2 = \Sigma[w(F_0^2-F_c^2)^2]/\Sigma[w(F_0^2)^2]^{1/2}$