Electronic Supplementary Material (ESI) for Dalton Transactions


**Supplementary Information**

# Correlation between slow magnetic relaxation and coordination structures of family of linear trinuclear Zn(II)-Ln(III)-Zn(II) complexes (Ln = Tb, Dy, Ho, Er, Tm, and Yb)

Moe Maeda, Shiori Hino, Kei Yamashita, Yumiko Kataoka,
Motohiro Nakano, Tomoo Yamamura, and Takashi Kajiwara*

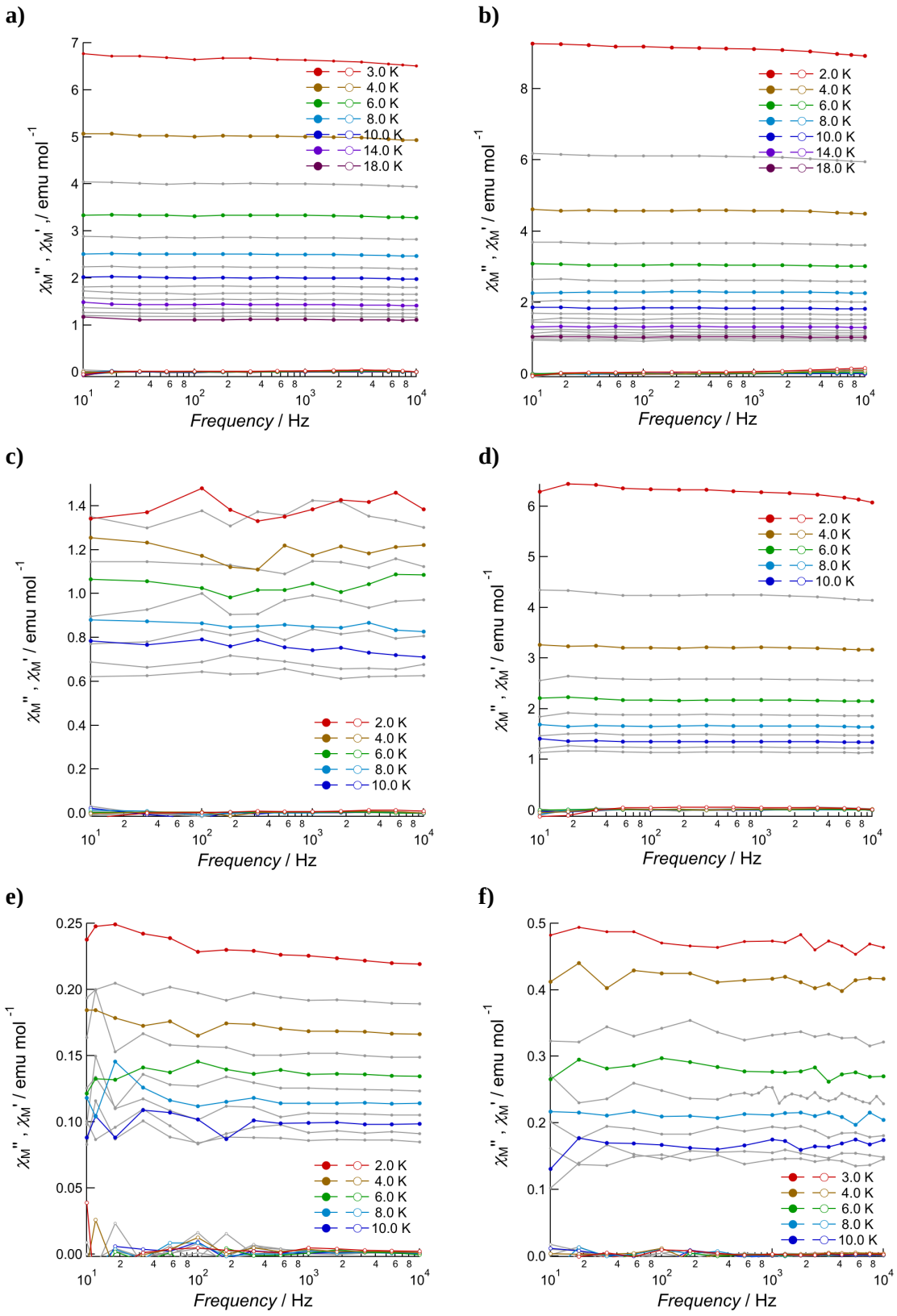


**Fig. S1**. Frequency dependence of the AC susceptibility data for a) **1**, b) **2**, c) **3**, d) **4**, e) **5**, and f) **6**, measured under zero DC field. Closed circles and open circles represent the in-phase ($\chi_M$') and out-of-phase ($\chi_M$'') components of the molar AC susceptibilities, respectively. Solid lines are provided for ease of viewing.

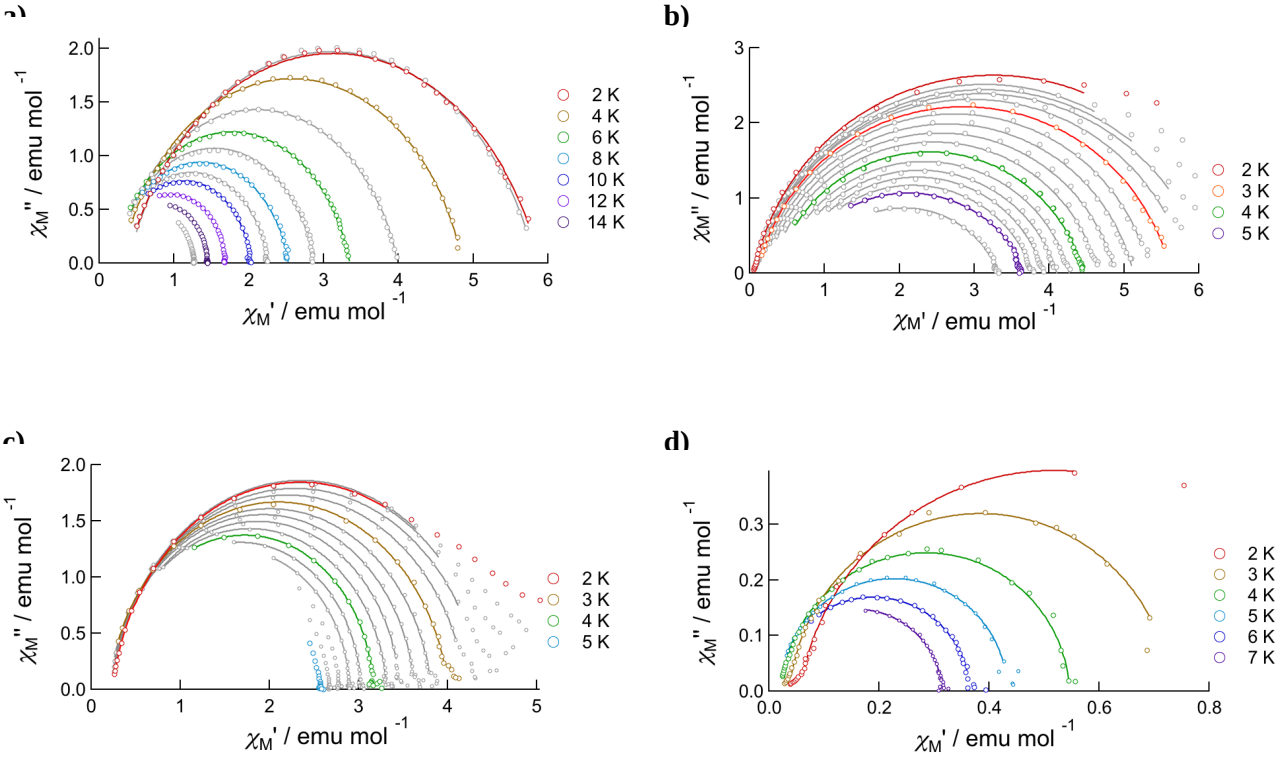


**Fig. S2**. Cole–Cole plots for a) **1**, b) **2**, c) **4**, and d) **6**, measured under 1000 Oe external DC field. The solid curves are theoretical calculations on the basis of generalized Debye equations. $\alpha$ parameters were estimated as 0.062–0.240 (2.0–12.0 K) for **1**, 0.014–0.118 (2.2–7.0 K) for **2**, 0.142–0.253 (2.2–4.0 K) for **4**, and 0.0143–0.111 (2.4–6.0 K) for **6**, respectively.

**Detail of the DFT calculation**

The DFT calculation was performed with the Gaussian 03, Revision E.01. (M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.).

Model complexes including La ($4f^0$) or Lu ($4f^{14}$) were employed for the calculation to investigate the influence of the different Ln ions as well as basis sets, for which the atomic coordinates of the complex **6** were used in a single-point calculation. Usual LanL2DZ basis set (for $4f^0$ system) as well as CEP-121G Stevens/Basch/Krauss ECP triple split basis set (for both systems: W. Stevens, H. Basch, J. Krauss, *J. Chem. Phys*. **1984**, *81*, 6026; W. J. Stevens, M. Krauss, H. Basch, P. G. Jasien, *Can. J. Chem*. **1992**, *70*, 612; T. R. Cundari, W. J. Stevens, *J. Chem. Phys*. **1993**, *98*, 5555) were used; for the latter, 5D and 7F keywords were assigned for pure d and f functions. Convergence of electronic states was achieved under the QC option. Population analyses were carried out to obtain the Mulliken charge on each atom which is summarized below. The results show slight difference in the absolute values of Mulliken charges, however, the normalized values, which were defined as the largest negative charge to be –1 given in parentheses, show similarity.

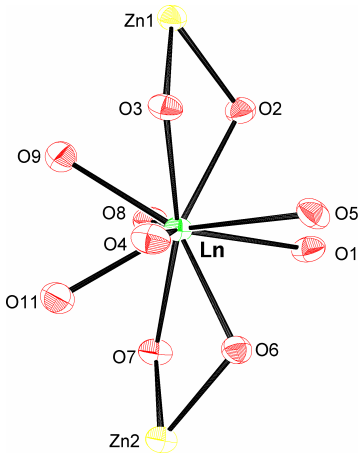


**Table S1** Estimated Mulliken charges calculated for Ln = La and Lu, using different basis functions. Normalized charges were given in parentheses.

| | La; B3LYP/LanL2DZ | La; B3PW91/CEP-121G | Lu; B3PW91/CEP-121G |
|---|---|---|---|
| O1 | –0.41 (–0.59) | –0.33 (–0.57) | –0.29 (–0.52) |
| O4 | –0.35 (–0.51) | –0.23 (–0.39) | –0.19 (–0.33) |
| O5 | –0.41 (–0.59) | –0.34 (–0.59) | –0.31 (–0.54) |
| O8 | –0.37 (–0.54) | –0.27 (–0.46) | –0.21 (–0.38) |
| | Av. –0.39 (–0.56) | Av. –0.29 (–0.50) | Av. –0.25 (–0.44) |
| O2 | –0.66 (–0.96) | –0.51 (–0.89) | –0.49 (–0.87) |
| O3 | –0.68 (–0.99) | –0.55 (–0.95) | –0.53 (–0.94) |
| O6 | –0.69 (–1.00) | –0.58 (–1.00) | –0.56 (–1.00) |
| O7 | –0.67 (–0.96) | –0.54 (–0.93) | –0.52 (–0.92) |
| | Av. –0.68 (–0.98) | Av. –0.55 (–0.94) | Av. –0.53 (–0.93) |
| O9 | –0.43 (–0.62) | –0.34 (–0.59) | –0.31 (–0.56) |
| O11 | –0.42 (–0.61) | –0.33 (–0.56) | –0.30 (–0.53) |
| | Av. –0.43 (–0.62) | Av. –0.34 (–0.58) | Av. –0.31 (–0.55) |