THE JOURNAL OF PHYSICAL CHEMISTRY Letters

Addition/Correction

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Correction to "Key Role of Frustration in Suppression of Magnetization Blocking in Single-Molecule Magnets"

Veacheslav Vieru, Liviu Ungur, and Liviu F. Chibotaru*

J. Phys. Chem. Lett. **2013**, *4*, 3565−3569. DOI: 10.1021/jz4017206

Supporting Information

The corrections refer only to the Supporting Information of the article.

(1) Figure S1 shows now only the results of ab initio calculations.

(2) The published atomic coordinates in the Supporting Information correspond now to the coordinates of the structures obtained using the AVOGADRO molecular mechanics program.[1]

The above corrections are caused by the fact that the previous atomic structures of compounds **1** and **2** had not been published at the moment of publication of the present Letter. Recently published magnetic measurements for compound **1** are in agreement with calculated magnetism.[2]

The above changes do not affect the main conclusion of our paper, namely, the incompatibility of magnetic blocking behavior (SMM) with the existence of magnetic frustration in the ground state, which emerges entirely from the ab initio analysis. Calculations on a series of different versions of structures of **1**, **2**, and **3** have shown that small deformations of the C_{80} core and small deformations of the Dy_3N unit do not modify the frustrated ground state of **3**, which give additional evidence for the above-mentioned conclusion.

■ ASSOCIATED CONTENT

Supporting Information

Computational details, details of the $DySc_2N$@C80 complex, the Dy_2ScN@C80 complex, and the electronic and magnetic properties of individual Dy centers, an account of the total magnetic interaction in the Dy_3N@C80 complex, the *xyz* coordinates of the investigated complexes, and the directions of the main magnetic axes of the ground KD of Dy ions. This material is available free of charge via the Internet at http://pubs.acs.org.

■ REFERENCES

(1) Hanwell, M. D.; Curtis, D. E.; Lonie, D. C.; Vandermeersch, T.; Zurek, E.; Hutchison, G. R. Avogadro: an Advanced Semantic Chemical Editor, Visualization, and Analysis Platform . *J. Cheminformatics* **2012**, *4*, 1−17, http://avogadro.cc/wiki/Main_Page.

(2) Westerström, R.; Dreiser, J.; Piamonteze, C.; Muntwiler, M.; Weyeneth, S.; Krämer, K.; Liu, S.-X.; Decurtins, S.; Popov, A.; Yang, S.; Dunsch, L.; Greber, T. Tunneling, Remanence, and Frustration in Dysprosium-Based Endohedral Single-Molecule Magnets. *Phys. Rev. B* **2014**, *89*, 060406.

Published: April 28, 2014