Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Magneto-optical investigations of molecular nanomagnet monolayers

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1. Oxidation of $(NBu_4)[DyPc_2]$ in chloroform

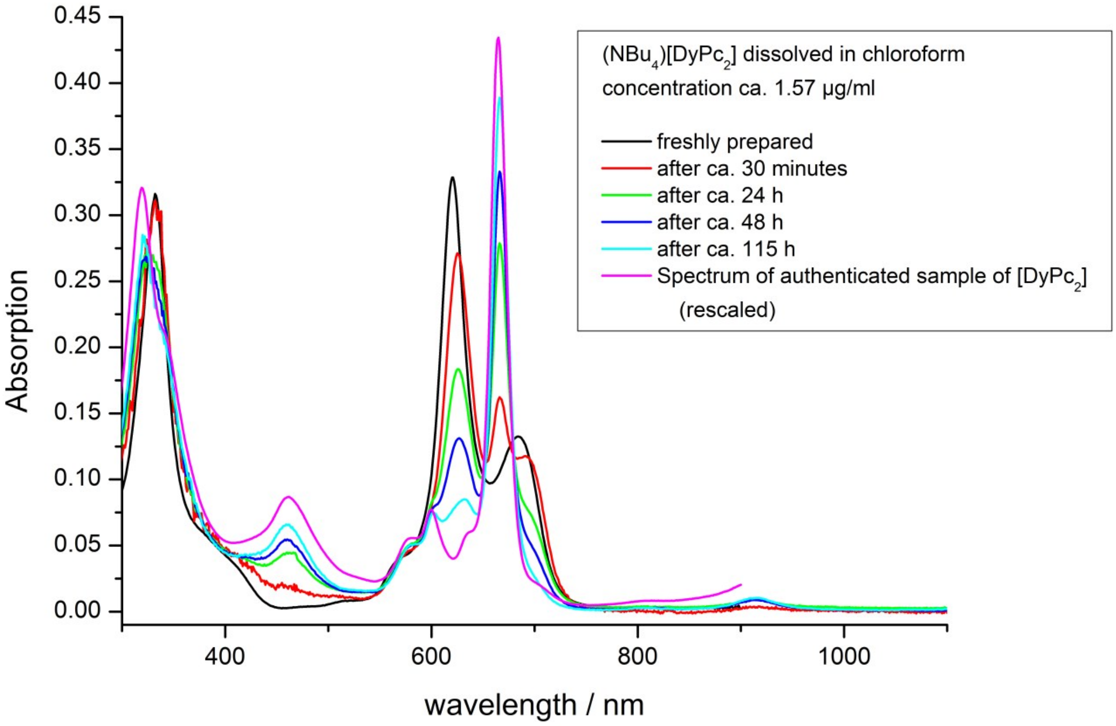

Figure S1 UV/Vis spectra of a solution of $(NBu_4)[DyPc_2]$ in chloroform recorded in a closed cuvette as a function of time as indicated in the figure.

2. XPS analysis of $DyPc_2$ film on quartz substrate

X-ray photoelectron spectra measured on a sample with $DyPc_2$ monolayer prepared by Langmuir-Blodgett technique are presented in Fig. S2. In addition to peaks associated with quartz substrate (Si and O) and carbon contamination layer (a part of the C 1s intensity) we observe rather weak but clear signal related to $DyPc_2$ molecules. Position and FWHM of the Dy $5d_{5/2}$ peak is consistent with the one expected for Dy(III). [S1, S2] More intriguing is the observation of two distinct peaks in N 1s spectrum. For phthalocyanines, only the peak possessing a lower binding energy (BE) is observed in the intact bulk phase. However, both observed peaks are frequently observed for phthalocyanine layers [S3, S4]. The lower binding energy peak refers to N atoms that contribute to the π system with one p electron, while the higher BE refers to N atoms with two p electrons in the π system. The presence of the higher BE peak could be caused by (i) hydrogenation of N atoms in phthalocyanine, “pyrrolic”-type nitrogen (although not necessarily coordinated in a pentagonal arrangement as pyrrole), or (ii) bonding to oxygen atom.[S3, S4] Additionally, for a thicker $DyPc_2$ layer we observe that only the lower BE peak increase in its intensity. Hence, we infer that this component is related to the phthalocyanine bonding to the substrate or specific intermolecular bonding in the first phthalocyanine layer. However, further systematic experiments are required to understand the origin of the higher BE peak.

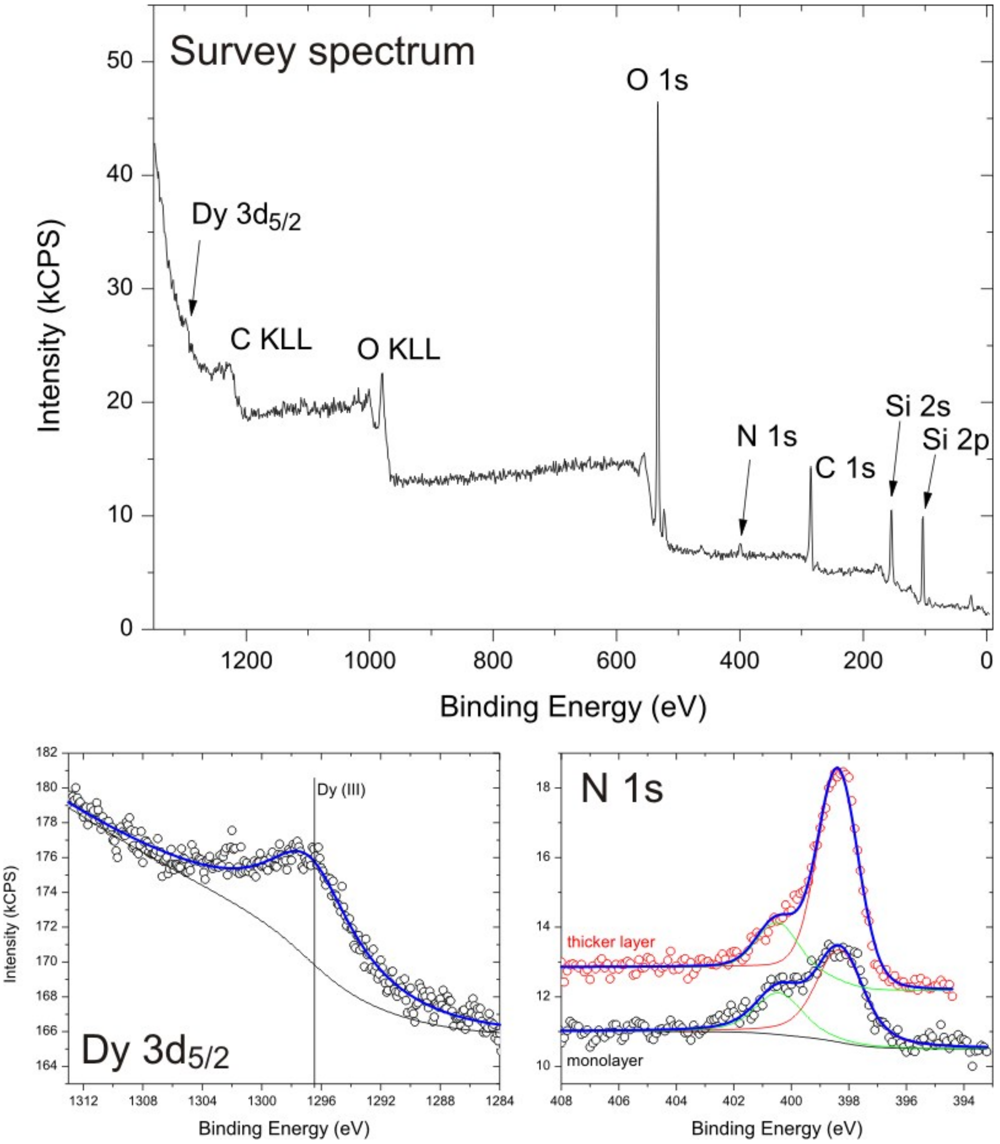

Figure S2 XPS Survey and detailed Dy $3d_{5/2}$ and N 1s spectra recorded on a Langmuir-Blodgett monolayer of 1 on quartz. For comparison, the N 1s peak, measured on a thicker $DyPc_2$ layer, is also shown.

2. References

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S3 S. Maldonado and K. J. Stevenson, *J. Phys. Chem. B*, 2004, **108**, 11375-11383.

S4 Y. Bai, F. Buchner, M. T. Wendahl, I. Kellner, A. Bayer, H.-P. Steinrück, H. Marbach, J. M. Gottfried, *J. Phys. Chem. C* 2008, **112**, 6087-6092.