Abstract Submitted
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Magnetic Relaxation Mechanisms in Lanthanide Single Molecule Magnets LIVIU CHIBOTARU, LIVIU UNGUR, University of Leuven, ERIC MCINNES, RICHARD WINPENNY, University of Manchester, UNIVERSITY OF MANCHESTER COLLABORATION — *Ab initio* investigation of multiplet spectrum of lanthanides in archetypal coordination geometries shows an unexpected regular structure consisting of (*i*) mirror symmetry of anisotropic magnetic properties of doublet states, (*ii*) high magnetic axiality of low-lying and high-lying doublets, comparable to complexes with ideal axial symmetry, and (*iii*) the strong rotation of the anisotropy axes of individual doublets [1]. The obtained high axiality of the ground doublet states explains the SMM behaviour of low-symmetry lanthanide complexes. *Ab initio* calculations predict that depending on the relative orientation of anisotropy axes in different doublet states, the relaxation can proceed via the first or the second excited state. Here we report new lanthanide cage complexes where two competing relaxation pathways through the first and second excited states are observed, leading to very high energy barriers for loss of magnetisation [2]. [1] L. Ungur, L.F. Chibotaru, *P.C.C.P.*, **2011**, *13*, 20086–20090. [2] R.J. Blagg, L. Ungur, F. Tuna, D. Collison, E.J.L. McInnes L.F. Chibotaru, R.E.P. Winpenny,. *Nat. Chem.*, submitted.

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