DFT Magnetic Characterization of a Fe_4 SMMs Series: From Isotropic Exchange Interactions to Multi-Spin Zero Field Splitting.

Supplementary Information Materials

Isotropic Exchange Coupling Constants

From Table 1, it is evident that the differences among the computed three J_1 values are small and this results support their supposed experimental equivalence by symmetry. Moreover, it comes also out that calculations suggest as more appropiate axial C_2 symmetry than a C_3 one.

Table 1 Calculated PBE0 Exchange Coupling Constants J_1

	Fe_4OMe	Fe_4tBu	Fe_4Ph	Fe_4Me	Fe_4C5	Fe_4C4	Fe_4C3	Fe_4C1
$J_1^{'}$	23.53 cm^{-1}	22.05 cm^{-1}	13.28 cm^{-1}	16.60 cm^{-1}	17.39 cm^{-1}	15.44 cm^{-1}	13.17 cm^{-1}	11.58 cm^{-1}
$J_1^{''}$	23.31 cm^{-1}	22.04 cm^{-1}	12.97 cm^{-1}	16.41 cm^{-1}	15.25 cm^{-1}	11.60 cm^{-1}	10.68 cm^{-1}	12.20 cm^{-1}
$J_1^{'''}$	23.25 cm^{-1}	22.04 cm^{-1}	13.06 cm^{-1}	16.39 cm^{-1}	15.25 cm^{-1}	10.85 cm^{-1}	9.40 cm^{-1}	13.47 cm^{-1}

PBE v.s. PBE0 Single Ion Anisotropy Tensors for Fe_4Ph

Table 2 Calculated Single Ion Anisotropy Tensors and their orientations.

	D[a]			E/D[a]			XC functional
	Fe_c	Fe_p [b]	$Fe_{p'}$ [b]	Fe_c	Fe_p [b]	$Fe_{p'}$ [b]	
Fe_4Ph	-0.307	0.841	0.841	~ 0	0.062	0.080	PBE
Fe_4Ph	0.225	-0.242	0.152	0.320	0.319	0.254	PBE0

[a] Values expressed in cm^{-1};
[b] Fe_p refers to the peripheral Iron laying on the $\mathbf{C_2}$ and $Fe_{p'}$ refers to Irons which do not;