

## Linking $[M^{III}_3]$ triangles with “double-headed” phenolic oximes

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### Supplementary Information:

#### Fitting of the magnetic data of 1:

The fitting of the magnetic data of **1** within the model introduced in the main article is *not* unique. The Table below reports the different regions of the parameters space where it is possible to find acceptable fits. To better understand the relationships between inter- and intra-triangle parameters, the exchange constant  $J_1$  is taken as a reference and the other parameters are reported as ratios of  $J_1$  (see inset of Figure 9).

In order to have a low-spin ground multiplet ( $S = 1/2$  or  $S = 3/2$ ) as suggested by the low-T value of  $\chi T$ ,  $J_3/J_1 < 2$  is required. Due to the small structural differences within each triangle, we have constrained the ratios between intra-triangle constants  $J_2/J_1$  and  $J'_2/J_1$  between 0.5 and 2.

	$J_1$	$J_3/J_1$	$J_2/J_1$	$J'_2/J_1$
<b>Region 1</b>	30 - 36 $\text{cm}^{-1}$	1.1 - 1.4	1.7 - 2	1.7 - 1.2
<b>Region 2</b>	47 - 70 $\text{cm}^{-1}$	0.6 - 0.9	0.8 - 1.3	0.8 - 1.2
<b>Region 3</b>	100 - 120 $\text{cm}^{-1}$	0.2	1.7 - 1.8	0.6 - 0.7
<b>Region 4</b>	50 - 70 $\text{cm}^{-1}$	0.4 - 0.6	1 - 1.6	0.5 - 0.8
<b>Region 5</b>	40 - 55 $\text{cm}^{-1}$	0.5 - 0.6	0.9 - 1.4	1.6 - 2
<b>Region 6</b>	90 - 110 $\text{cm}^{-1}$	0.2 - 0.3	0.5	0.6 - 0.8
<b>Region 7</b>	70 - 90 $\text{cm}^{-1}$	0.2	1.2 - 1.3	0.8 - 1.3

In all the regions it is possible to adjust parameters and ratios in order to fit both susceptibility and magnetization data. The set of parameters reported in the main article belongs to region 2, where there is the best overall agreement between the values of the exchange constants and the expectations based the model of Cañada-Vilalta *et al.*<sup>1</sup>

1 C. Cañada-Vilalta, T. A. O'Brien, E. K. Brechin, M. Pink, E. R. Davidson and G. Christou, *Inorg. Chem.*, 2004, **43**, 5505.