

A Unique Single Carboxylate-Bridged Spin-Frustrated Chiral Mn(II) Metallatriangle

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Supplementary material

Table S1: SHAPE output for the evaluated structures

Structure reference	CSD	Pentagonal bipyramid	Capped octahedron	Capped trigonal prism
AXIREE		0.91438	8.16263	6.53529
FIGGAE		0.82747	8.02865	6.42132
FIQSOO		1.00119	5.76113	4.40102
FIQTAB		0.99804	7.22245	5.73491
GIHQEU		0.87975	7.77166	6.24538
GIHQIY(I) ^a		1.36376	5.77637	4.44913
GIHQIY(II) ^a		0.81174	6.32173	4.94905
JAGRAL		0.96025	7.88047	6.61806
LOSDAZ		1.63227	5.94122	4.59629
MANRAV		0.52648	6.72175	5.20232
MANRID		0.53119	7.46056	5.84117
MIGZEI		0.68803	6.83953	5.28132
ODOTIL		0.78826	7.28595	5.70130
OFOGEW		0.88657	5.73824	4.31532
PEKNEZ		0.92749	7.23441	5.90991
QOJXUJ		0.59710	6.50373	5.31950
QOJYaq		0.53304	6.83747	5.47998
QOJYEU		0.50715	6.77385	5.41593
RAHBIM		0.41847	6.96780	5.62434
SEPPUZ		0.92757	6.20869	4.74620
WOCHOM		1.19231	7.15811	6.11708
XAZKUF		0.73651	8.06748	6.58187
XEGDIW		1.03871	5.96994	4.55886

^a Two different coordination polyhedra can be found for this structure

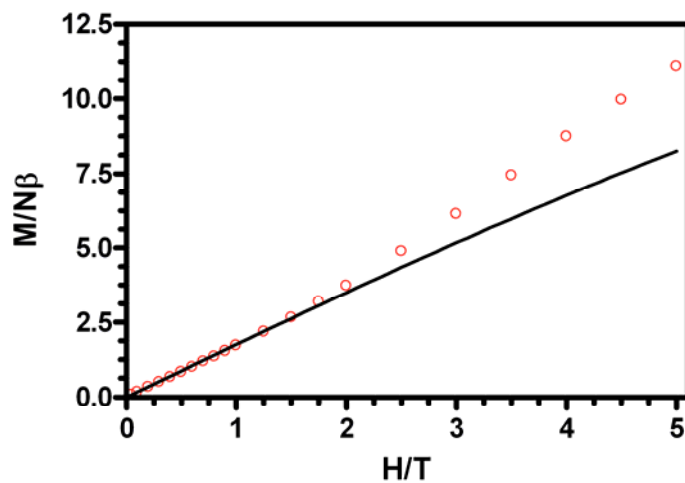


Figure S1.- Experimental M vs H plot at 2K. The line corresponds to the simulation of the M vs H data with the parameters: $J=-0.17\text{ cm}^{-1}$, $g=2.046$, $D=3.17\text{ cm}^{-1}$ and $E=0.76\text{ cm}^{-1}$

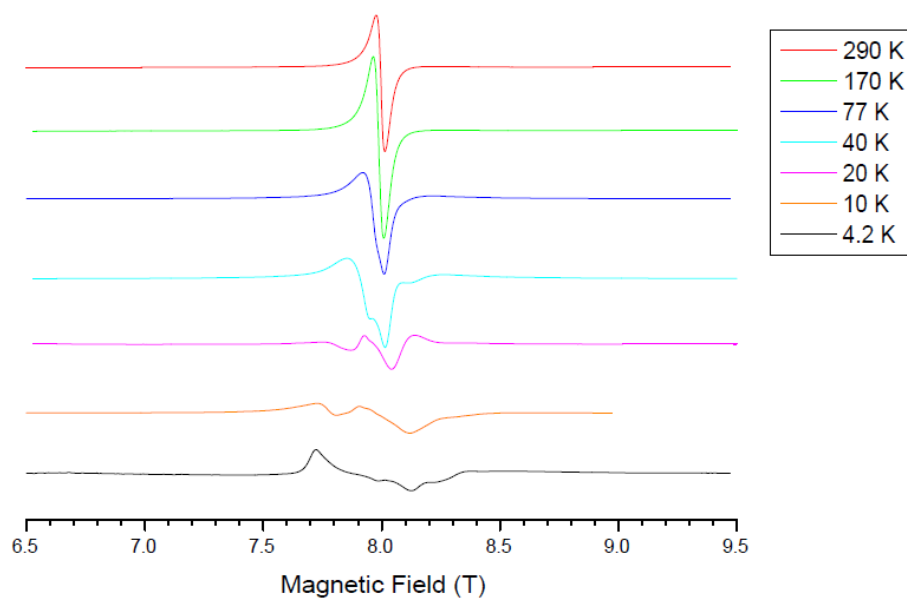


Figure S2.- Temperature dependence of the HFEPR spectrum of **1** at 224GHz