

Electronic Supplementary Information (ESI) for

" Chiroptical and magnetic properties of star-shaped Fe^{III}_4 complexes from chiral Schiff bases. Structural and magnetic correlations based on continuous shape measurements "

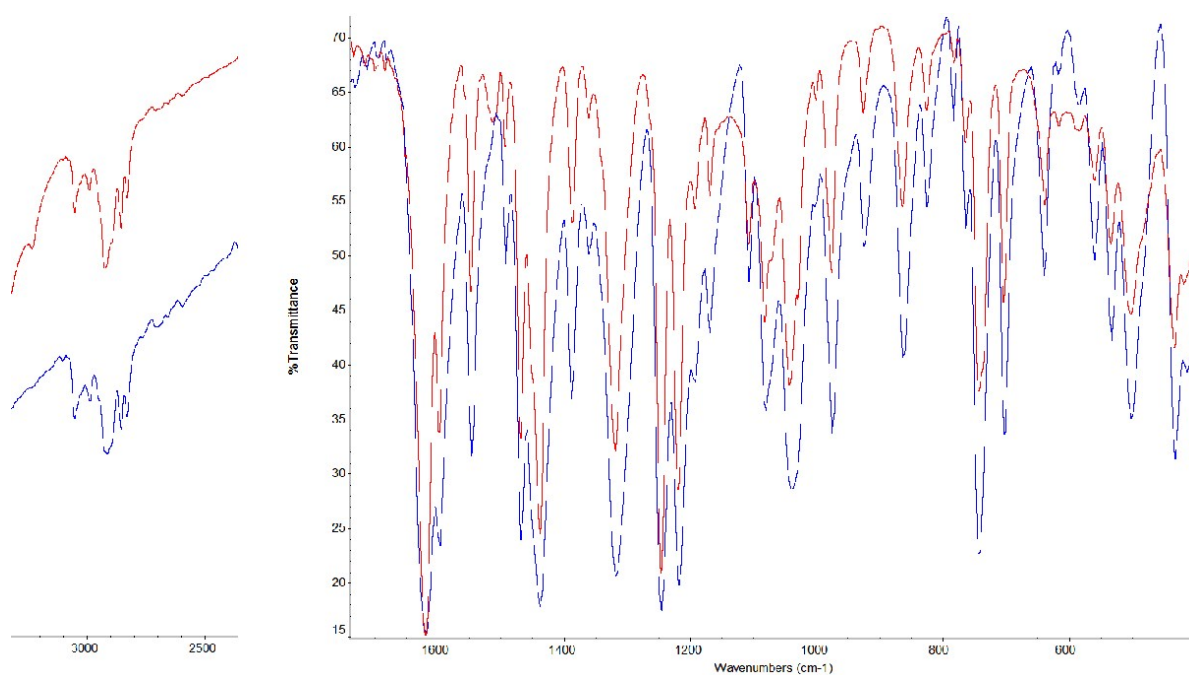


Fig S1. IR spectra for the enantiomers of **1R** (red) and **1S** (blue).

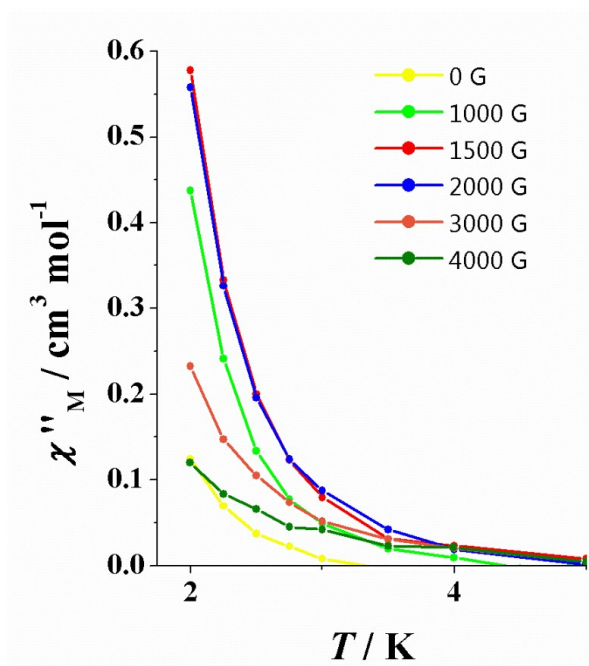


Fig S2. AC response of the under different static fields and at the 1000 Hz frequency for complex **1R**. From these data the 1500 G field was selected for the alternate current measurements.

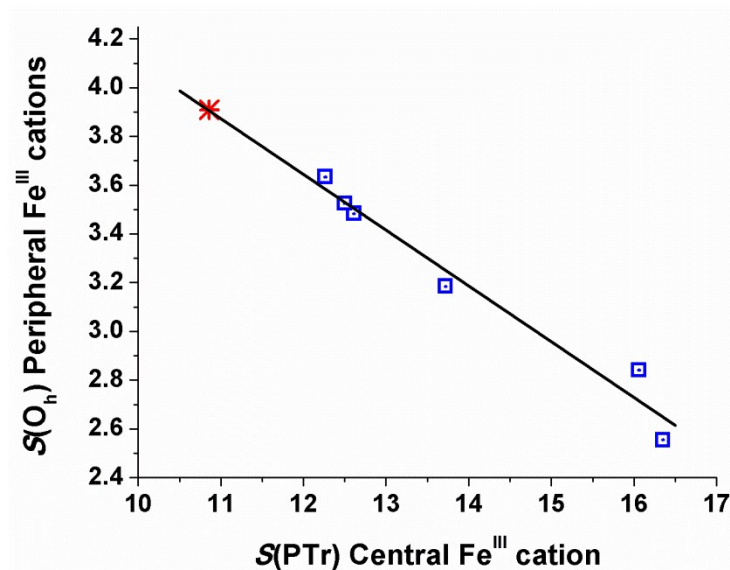


Fig S3. $S(\text{PTTr})$ for the central Fe^{III} cations versus $S(\text{O}_h)$ for the peripheral ones, showing the correspondence between both distortions for the reported complexes type **VI**. (Red star shows the values for complex **1S** that shows the larger distortion from the regular polyhedra.

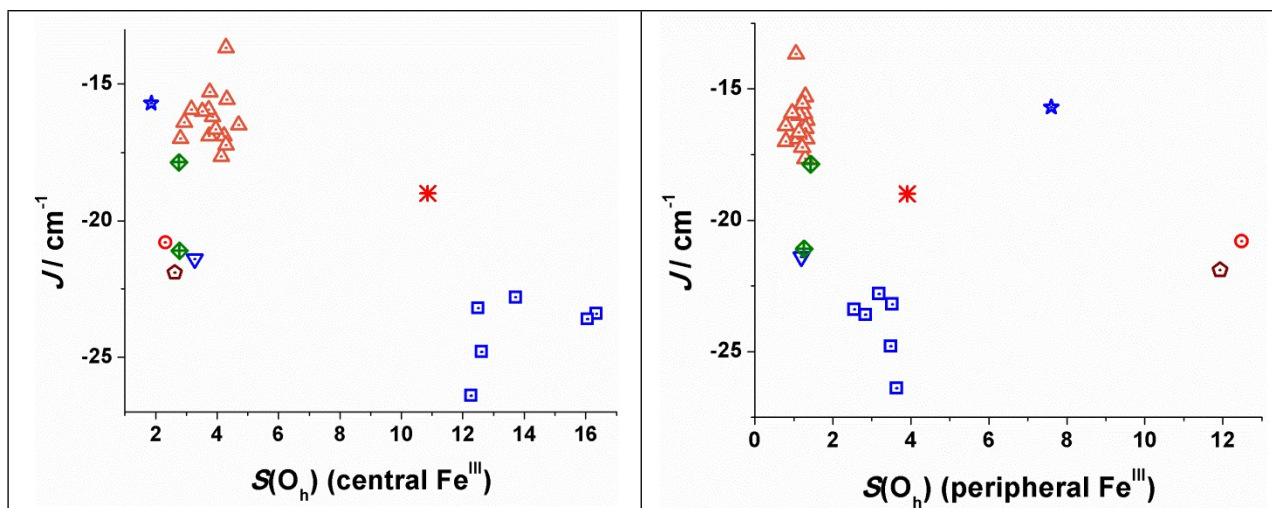


Fig S4 $S(\text{O}_h)$ vs. J for all the reported Fe_4 complexes. Any direct correlation can be extracted between the distortion of the central or peripheral environments and the magnitude of the interaction. However, each type of complexes shows a range of characteristic values.

Table S1. Selected bond distances (Å) and angles (°) for the core of compound **2RS**.

Fe1-O1	1.901(2)	Fe1-O5	1.931(2)
Fe1-O2	1.963(2)	Fe1-N1	2.137(2)
Fe1-O4	2.206(2)	Fe1-N2	2.128(2)
O1-Fe1-O2	161.22(7)	O4-Fe1-O5	154.56(7)
O1-Fe1-O4	95.76(7)	O4-Fe1-N1	92.23(7)
O1-Fe1-O5	99.53(8)	O4-Fe1-N2	73.90(7)
O1-Fe1-N1	78.31(8)	O5-Fe1-N1	110.66(8)
O1-Fe1-N2	91.09(8)	O5-Fe1-N2	85.55(8)
O2-Fe1-O4	83.07(7)	N1-Fe1-N2	161.75(8)
O2-Fe1-O5	88.70(7)		
O2-Fe1-N1	82.99(8)		
O2-Fe1-N2	106.45(8)		

Table S2. Fit values for the τ_0 and U_{eff} parameters from the $\ln(\chi''/\chi')$ vs. $1/T$ plots.

Frequency (Hz)	τ_0	U_{eff}
1488.1	7.02 E-07	10.22
1320.4	5.61 E-07	10.68
1143.3	4.77 E-07	11.03
997.3	5.06 E-07	10.96
852.3	5.24 E-07	10.94
679.3	5.19 E-07	11.02
509.5	6.02 E-07	10.81
349.8	8.29 E-07	10.31

Table S3 $S(O_h)$ and $S(PTr)$ values calculated for the central and peripheral cation of the reported Fe_4 star-shaped systems.

CCDC	Type	Central Fe^{III}		Peripheral Fe^{III}						Peripheral Fe^{III}	
		$S(O_h)$	$S(PTr)$	$S_1(O_h)$	$S_1(PTr)$	$S_2(O_h)$	$S_2(PTr)$	$S_3(O_h)$	$S_3(PTr)$	Mean $S(O_h)$	Mean $S(PTr)$
AGAQIJ	I	3.849	5.630	1.263	10.096	1.274	10.006	1.445	9.557	1.327	9.886
DOPKAV	I	3.114	6.488	1.120	10.559	0.868	11.381	0.696	12.199	0.895	11.380
DUFNUO	I	2.809	7.149	0.991	11.613	0.601	13.051			0.796	12.332
DUFPAW	I	2.936	6.860	0.958	11.876	0.623	12.875			0.790	12.375
DUPSAK	I	3.727	5.658	1.382	10.119	1.149	10.358			1.265	10.239
ICOCIN	I	3.767	5.619	1.443	10.081	1.130	10.430			1.287	10.255
ITAKUJ	I	4.701	4.676	1.295	10.102					1.295	10.102
KAXGUN	I	3.746	5.644	1.141	10.627	1.061	10.632			1.101	10.630
NIPJEC	I	4.228	5.161	1.346	9.674	1.286	10.163			1.316	9.919
TACFUA	I	4.292	4.990	1.005	10.822	1.105	10.634			1.055	10.728
TACGAH	I	3.957	5.396	1.380	9.613	0.873	11.646			1.127	10.629
VOBXUG	I	3.520	5.983	1.226	10.391	1.050	10.768			1.138	10.580
XUBVUM	I	4.140	5.254	1.576	9.171	1.093	10.725	1.207	10.210	1.292	10.036
XUBWAT	I	4.294	5.043	1.395	9.577	1.033	11.023			1.214	10.300
XUBWEX	I	4.317	5.026	1.405	9.581	1.036	11.026			1.220	10.304
XUBWIB	I	3.167	6.414	0.921	11.156	0.992	11.060			0.956	11.108
ICOCOT	II	3.277	7.523	1.193	11.619					1.193	11.619
DEKPAK	III	2.780	8.687	1.413	10.391	1.113	12.439			1.263	11.415
GANWEA	III	2.766	8.882	1.630	9.762	1.229	11.867			1.430	10.814
ABOKIL	IV	2.449	9.947	11.733	3.734	10.817	4.824			11.275	4.279
ABOLEI	IV	2.400	9.858	12.439	3.632	12.606	3.094			12.522	3.363
MEMKAR	IV	2.318	10.452	14.082	3.413	11.412	3.981	11.953	3.190	12.482	3.528
SAGBOU	IV	2.654	9.572	13.013	3.816	11.868	3.911	11.790	4.008	12.224	3.912
CUHJEW	V	1.859	12.764	5.124	5.882	9.085	2.769	8.593	2.919	7.601	3.857
TACHIR	V	1.792	13.075	6.953	4.008	6.617	4.035	8.570	3.298	7.380	3.780
JORWAQ	VI	16.350	0.466	2.554	9.721					2.554	9.721
UVIPUL	VI	16.059	0.550	2.800	9.166	3.114	9.172	2.608	9.559	2.841	9.299
XOKDEI	VI	12.611	0.975	3.444	8.048	3.725	7.148	3.283	8.419	3.484	7.872
XOKDIM	VI	12.502	0.987	3.913	6.941	3.262	8.389	3.401	8.032	3.525	7.787
XOKDOS	VI	12.266	1.094	3.668	7.857	4.273	7.018	2.961	8.416	3.634	7.763
XOKQAR	VI	13.718	0.790	3.332	8.486	3.087	8.528	3.134	8.819	3.184	8.611
1S	VI	10.861	1.618	4.082	7.147	2.421	9.530	5.225	6.318	3.909	7.665
AHOTEX	VII	2.624	10.588	11.628	6.205	11.684	6.228	12.476	6.001	11.929	6.144
DAMREQ	VIII	0.843	15.123	3.305	6.029	2.844	6.771			3.074	6.400
GAGREM	VIII	5.888	3.855	1.284	13.660	1.270	13.577			1.277	13.619

LEBRIU	VIII	3.234	8.247	3.078	7.170	PyQ*	PyQ*	3.078	7.170
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* Square pyramidal environment.