An unprecedented trinuclear structure involving two high-spin and one spin-crossover iron(II) centres

George Psomas, Nicolas Bréfuel, Françoise Dahan, and Jean-Pierre Tuchagues*
Laboratoire de Chimie de Coordination, UPR CNRS 8241, 205 route de Narbonne, 31077 Toulouse, France

Supporting Information Available: Mössbauer parameters obtained from fitting the Mössbauer spectra (80-300 K) of complex **1** (Table SI-1). Magnetic data (Table SI-2) and temperature dependence of the $\chi_M T$ product (Figure SI-1). X-ray crystallographic file of $Fe_3L_2(SCN)_4(H_2O)$ (**1**), in CIF format. This material is available free of charge via the Internet at http://pubs.acs.org.

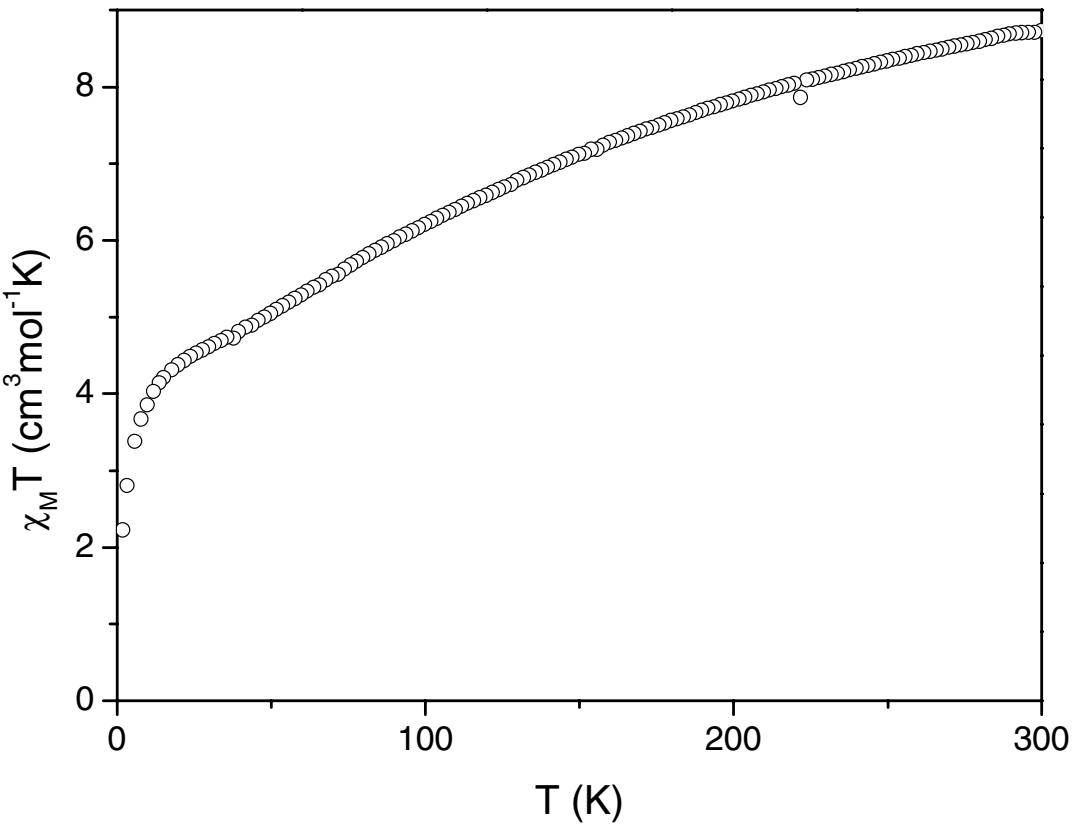

Figure SI-1. Temperature dependence of the $\chi_M T$ product of complex **1**.

Table SI-1. Mössbauer parameters of complex **1**and their standard deviations of statistical origin (given in parentheses).

Site	T (K)	Area ratio (%)	δ (mm/s)	ΔE_Q (mm/s)	Γ/2 (mm/s)
Fe1 (LS)	80	32.01(41)	0.334(3)	1.320(7)	0.130(7)
	100	33.90(56)	0.327(6)	1.326(10)	0.139(4)
	120	32.60(58)	0.321(6)	1.323(12)	0.133(5)
	140	31.68(83)	0.314(6)	1.321(12)	0.132(5)
	160	30.26(87)	0.311(6)	1.311(12)	0.127(6)
	180	27.5(10)	0.291(13)	1.33(3)	0.127(8)
	200	25.95(81)	0.282(12)	1.34(3)	0.138(6)
	220	22.96(94)	0.281(21)	1.33(4)	0.145(10)
	240	20.1(10)	0.271(29)	1.29(6)	0.155(13)
	260	21.1(14)	0.263*	1.22(3)	0.23(2)
	280	18.0(21)	0.255*	1.18(5)	0.21(3)
	300	22.6(25)	0.248*	1.18(7)	0.29(4)
Fe1+Fe3 (HS)	80	34.65(58)	1.008(4)	2.795(6)	0.144(4)
	100	33.77(91)	1.004(5)	2.779(9)	0.141(6)
	120	34.06(91)	0.992(6)	2.76(1)	0.143(6)
	140	34.98(94)	0.983(5)	2.75(1)	0.141(6)
	160	36.4(10)	0.968(5)	2.72(1)	0.138(5)
	180	39.1(14)	0.962(12)	2.68(3)	0.142(7)
	200	40.7(10)	0.942(8)	2.65(2)	0.136(5)
	220	43.7(11)	0.927(8)	2.62(2)	0.141(5)
	240	46.6(13)	0.914(7)	2.60(2)	0.143(4)
	260	45.6(12)	0.897(6)	2.57(1)	0.146(6)
	280	48.7(21)	0.882(10)	2.51(1)	0.145(8)
	300	44(22)	0.870(10)	2.47(2)	0.135(9)
Fe2 (HS)	80	33.33*	1.160(3)	2.808(6)	0.159(4)
	100	33.33*	1.152(4)	2.805(8)	0.162(7)
	120	33.33*	1.142(4)	2.800(7)	0.159(6)
	140	33.33*	1.136(5)	2.791(9)	0.162(5)
	160	33.33*	1.121(5)	2.775(10)	0.163(6)
	180	33.33*	1.105(8)	2.75(1)	0.165(9)
	200	33.33*	1.091(5)	2.744(10)	0.158(6)
	220	33.33*	1.074(8)	2.74(2)	0.167(7)
	240	33.33*	1.060(14)	2.72(3)	0.177(8)
	260	33.33*	1.028(10)	2.71(2)	0.175(9)
	280	33.33*	1.00(2)	2.60(4)	0.195(19)
	300	33.33*	0.98(2)	2.57(4)	0.19(2)

* fixed value.

Table SI-2. Magnetic data of complex **1** corrected for the diamagnetic contributions of the capsule and sample.

T (K)	χ_M (cm^3mol^{-1})	$\chi_M T$ ($cm^3mol^{-1}K$)	T (K)	χ_M (cm^3mol^{-1})	$\chi_M T$ ($cm^3mol^{-1}K$)
299.96	0.02911	8.73184	149.76	0.04752	7.13355
297.78	0.02925	8.71006	147.78	0.04791	7.1166
295.68	0.02946	8.71073	145.79	0.04837	7.08014
293.58	0.02965	8.70465	143.78	0.04879	7.05186
291.63	0.02983	8.69932	141.8	0.04925	7.01503
289.65	0.03	8.6895	139.81	0.04972	6.98365
287.75	0.03015	8.67566	137.8	0.05019	6.95135
285.77	0.0303	8.65883	135.8	0.05071	6.91618
283.79	0.03042	8.63289	133.81	0.05119	6.88642
281.84	0.03056	8.61303	131.8	0.05171	6.84973
279.78	0.03071	8.59204	129.81	0.05224	6.81538
277.81	0.03087	8.57599	127.78	0.05264	6.78127
275.78	0.03104	8.56021	125.81	0.05321	6.72634
273.79	0.03121	8.54499	123.8	0.05379	6.69435
271.75	0.03139	8.53023	121.81	0.05438	6.6592
269.78	0.03156	8.51426	119.8	0.05498	6.62403
267.75	0.03173	8.49571	117.8	0.05563	6.5866
265.75	0.03191	8.48008	115.79	0.05627	6.55321
263.79	0.03208	8.46238	113.82	0.05693	6.5155
261.77	0.03227	8.44732	111.8	0.05762	6.47977
259.74	0.03245	8.42856	109.79	0.05832	6.44192
257.78	0.03263	8.41136	107.8	0.05905	6.40295
255.79	0.03281	8.39247	105.8	0.05979	6.36559
253.79	0.033	8.37507	103.82	0.06056	6.32578
251.78	0.03319	8.35658	101.81	0.06134	6.28734
249.79	0.03338	8.33799	99.81	0.06217	6.24503
247.77	0.03357	8.31764	97.8	0.06302	6.20519
245.76	0.03377	8.29932	95.78	0.06392	6.16336
243.73	0.03397	8.27951	93.81	0.06481	6.12226
241.77	0.03417	8.26128	91.8	0.0658	6.07983
239.76	0.03437	8.24055	89.81	0.06676	6.04044
237.77	0.03457	8.21971	87.82	0.0678	5.99572
235.76	0.03478	8.19973	85.79	0.06887	5.9542
233.76	0.03499	8.17926	83.82	0.06998	5.90836
231.77	0.03521	8.16062	81.81	0.07115	5.86572
229.77	0.03542	8.13845	79.82	0.07236	5.82078
227.76	0.03564	8.11737	77.81	0.07362	5.77578
225.73	0.03588	8.09919	75.81	0.07493	5.72837
223.77	0.03614	8.08705	73.8	0.07625	5.68044
221.77	0.03544	7.85953	71.82	0.07741	5.62725
219.75	0.03661	8.04505	69.78	0.07926	5.55959
217.79	0.03684	8.02338	67.8	0.08087	5.53076
215.79	0.03708	8.00149	65.79	0.08235	5.48299
213.78	0.03732	7.97827	63.82	0.08443	5.41781
211.76	0.03757	7.95582	61.8	0.08638	5.38832

209.77	0.03782	7.9335	59.82	0.08842	5.33828
207.76	0.03807	7.90942	57.79	0.09068	5.28928
205.77	0.03833	7.88716	55.8	0.09305	5.2404
203.75	0.03857	7.85864	53.81	0.09561	5.19219
201.78	0.03885	7.83915	51.81	0.09836	5.14477
199.76	0.03912	7.81461	49.82	0.1013	5.09603
197.75	0.03937	7.78542	47.8	0.1046	5.04677
195.78	0.03966	7.76463	45.81	0.1082	4.99988
193.79	0.03994	7.73997	43.82	0.1117	4.95664
191.76	0.04024	7.71642	41.8	0.1164	4.89469
189.78	0.04052	7.68989	39.37	0.1222	4.86552
187.79	0.04081	7.66371	37.78	0.125	4.81101
185.77	0.04111	7.637	35.79	0.1323	4.7225
183.78	0.04141	7.61033	33.75	0.139	4.73502
181.77	0.04171	7.58163	31.77	0.1465	4.69125
179.76	0.04205	7.55891	29.77	0.1549	4.65431
177.79	0.04236	7.53118	27.77	0.1646	4.61137
175.78	0.04269	7.50405	25.78	0.1757	4.57094
173.79	0.04299	7.47123	23.85	0.1882	4.52955
171.77	0.04336	7.44795	21.83	0.2031	4.48857
169.8	0.0437	7.42026	19.83	0.2208	4.43367
167.76	0.04407	7.39318	17.82	0.2421	4.37846
165.79	0.04441	7.36273	15.15	0.2782	4.31422
163.8	0.04477	7.33333	13.8	0.3002	4.21473
161.79	0.04515	7.30482	11.85	0.3399	4.14276
159.79	0.04553	7.27524	9.86	0.3911	4.02782
157.78	0.04589	7.24052	7.85	0.4675	3.85625
155.77	0.04613	7.18567	5.82	0.5807	3.66988
153.8	0.04671	7.184	3.21	0.8737	3.37967
151.81	0.04699	8.73184	1.98	1.124	2.80458