Structural effects on magnetic properties of some hexadentate ferric complexes in bulk materials or intercalated in lamellar $CdPS_3$ matrix

Sébastien Floquet[a], M. Carmen Muñoz[b], Eric Rivière[a], René Clément[a], Jean-Paul Audière[a] and Marie-Laure Boillot[a]*.

Supplementary Information

Table S1 : Atomic coordinates of [Fe(3,5-Cl_2-Sal_2Trien)]PF_6 (**1**) at 293 K

	x	y	z
FE1	0.250000	0.750000	0.008558
CL2	-0.174449	0.490579	0.267850
CL1	-0.074708	0.844462	0.175448
O1	0.109806	0.754427	0.075447
C2	0.068523	0.591037	0.111573
N2	0.132631	0.795940	-0.088747
C4	-0.047142	0.722394	0.169868
C5	-0.114078	0.661801	0.216953
N1	0.269577	0.898453	0.013246
C3	0.047817	0.692034	0.115654
C7	0.003348	0.527428	0.157899
C6	-0.085804	0.564001	0.209866
C10	0.177116	0.750976	-0.161851
C1	0.163140	0.550238	0.059832
C9	0.126412	0.898565	-0.094135
C8	0.166994	0.948939	-0.030108
P1	0.250000	0.250000	0.059279
F1	0.156633	0.167266	0.061803
F2	0.173318	0.301528	0.123915
F3	0.174912	0.302346	0.000250

Table S2 : Atomic coordinates of [Fe(3,5-Cl_2-Sal_2Trien)]ClO_4 (**3**) at 293 K

	x	y	z
FE1	0.500000	0.723167	0.250000
O1	0.468636	0.790722	0.113285
O2	0.736448	0.976568	-0.099123
N1	0.646436	0.722088	0.230495
C7	0.644294	0.824701	0.084387
N2	0.460010	0.642833	0.12015
HN2	0.500500	0.647700	0.044300
C8	0.694961	0.769265	0.164966
C1	0.535106	0.832375	0.060577
C3	0.560451	0.936239	-0.080209
C4	0.665716	0.929161	-0.052371
C6	0.708770	0.874431	0.027418
C2	0.494724	0.888163	-0.024485
C5	0.697106	1.026111	-0.200570
C9	0.708674	0.666128	0.305958
C10	0.347421	0.647979	0.074398
C11	0.499732	0.571437	0.175023
CL1	0.000000	0.848710	0.250000
O3	-0.043704	0.813878	0.141451
O4	0.077668	0.890699	0.209490

Table S3 : Atomic coordinates of [Fe(5-OMe-Sal$_2$Trien)]PF_6 **.** 0.5H_2O (**5**) at 293 K

	x	y	z
FE1	0.218017	0.230033	0.009205
O1	0.280511	0.320091	-0.032009
O3	0.104362	0.187637	-0.121059
O4	0.053348	-0.110321	-0.290632
N4	0.346508	0.151733	-0.006439
C21	-0.019505	0.085145	-0.224203
C15	0.323691	0.089764	-0.064030
C4	0.262635	0.556104	0.013560
N1	0.103943	0.305288	0.052996
O2	0.253629	0.636690	0.031743
C16	0.200667	0.068236	-0.134335
N3	0.365512	0.233603	0.168963
N2	0.141006	0.151028	0.094682
C18	0.077057	-0.036358	-0.242058
C7	0.193248	0.428201	0.028513
C3	0.339250	0.527295	-0.033924
C2	0.344934	0.448040	-0.047179
C1	0.274085	0.396112	-0.016241
C8	0.113909	0.380625	0.064055
C22	0.098329	0.115927	-0.157219
C17	0.193265	-0.008760	-0.179299
C10	0.013478	0.180266	0.071415
C11	0.218215	0.149013	0.210326
C9	0.016259	0.267828	0.095062
C12	0.306962	0.219033	0.246619
C20	-0.029716	0.009015	-0.265473
C6	0.191724	0.509637	0.047629
C14	0.472353	0.166953	0.069798
C5	0.322857	0.690368	-0.007173
C13	0.463946	0.174036	0.180320
C19	0.154669	-0.163120	-0.261914
P1	0.615424	0.092899	0.826642
F1	0.525765	0.153324	0.843321
F2	0.709851	0.038405	0.815528
F3	0.693100	0.104454	0.947579
F4	0.545765	0.097226	0.713830
F5	0.557174	0.028242	0.866593
F6	0.691092	0.158452	0.812214
O5	0.933556	0.011383	0.977232

Table S4 : Atomic coordinates of [Fe(5-OMe-Sal$_2$Trien)]ClO_4 (**7**) at 293 K

	x	y	z
Fe	−0.2500	0.7500	0.4962
Cl1	0.0707	0.6483	0.3216
Cl2	0.1801	1.0046	0.2290
Cl3	0.2500	0.7500	0.5580
C6	-0.0654	0.9021	0.3907
C5	0.0043	0.9650	0.3425
C3	0.1107	0.8314	0.2822
C7	-0.1577	0.9426	0.4458
N1	-0.2281	0.8944	0.4930
01	-0.1112	0.7382	0.4263
C1	-0.0483	0.8017	0.3846
N2	-0.3704	0.7889	0.5908
C4	0.0908	0.9292	0.2892
C2	0.0452	0.7699	0.3297
C10	-0.3228	0.7504	0.6654
O2	0.1542	0.7936	0.6053
C8	-0.3181	0.9460	0.5439
C9	-0.3941	0.8909	0.5872
03	0.1991	0.6827	0.5135

Table S5 : Least-squares planes (x,y,z in crystal coordinates) and deviations from them. The atoms used to define the planes are the four donor atoms except in case of **3** (Plane 3) for which the iron center is added.

Complex	Plane	
1	1	N(1) - O(1) - N(1)_$1 - N(2)_$1 - Fe(1) 8.4094x - 1.9948y + 10.4025z = 0.4387 [N(1), 0.1529; O(1), -0.1825; N(1)_$1, 0.1975; N(2)_$1, -0.1679; Fe(1), 0.2529]
	2	N(2) - N(2)_$1 - O(1)_$1 - O(1) - Fe(1) 1.5000x + 13.9447y - 0.0000z = 10.8335 [N(2), 0.3039; N(2)_$1, -0.3039; O(1)_$1, 0.2133; O(1), -0.2133; Fe(1), 0.0000]
	3	N(1) - N(2) - N(1)_$1 - O(1)_$1 - Fe(1) 8.4094x - 1.9948y - 10.4025z = 0.7738 [N(1), -0.1975; N(2), 0.1679; N(1)_$1, -0.1529; O(1)_$1, 0.1825; Fe(1), -0.2529]
3	1	N(1) - O(1) - N(1)_$1 - N(2)_$1 - Fe(1) 6.7225x - 1.0507y + 12.8695z = 3.9141 [N(2)_$1, 0.0333; N(1), -0.0424; O(1), 0.0452; N(1)_$1, -0.0361; Fe(1), 0.0034]
	2	N(2) - N(2)_$1 - O(1)_$1 - O(1) - Fe(1) 2.5187x + 13.5449y + 0.0000z=9.5290 [N(2), -0.1429; N(2)_$1, 0.1429; O(1)_$1, -0.1871; O(1), 0.1871; Fe(1), 0.0000]
	3	N(1) - O(1) - N(1)_$1 - N(2)_$1 - Fe(1) 6.7222x - 1.0503y + 12.8698z = 3.9153 [N(1), -0.0430; O(1), 0.0445; N(1)_$1, -0.0368; N(2)_$1, 0.0327; Fe(1), 0.0027]
5	1	N(1) - O(1) - N(4) - N(2) - Fe(1) 4.4753x + 3.3877y + 9.4117z = 2.0202 [N(1), -0.0214; O(1), 0.0197; N(4), -0.0168; N(2), 0.0185; Fe(1), -0.1784]
	2	O(3) - N(4) - N(3) - N(1) - Fe(1) 6.3345x + 12.8921y - 7.7499z = 4.1053 [O(3), -0.0860; N(4), 0.0978; N(3), -0.0869; N(1), 0.0751; Fe(1), 0.1697]
	3	N(2) - N(3) - O(1) - O(3) - Fe(1) -8.6235x + 11.4256y + 5.9162z = 0.7902 [N(2), 0.2781; N(3), -0.2740; O(1), 0.2565; O(3), -0.2607; Fe(1), 0.0121]
7	1	N(1) - N(2) - N(1)_$1 - O(1)_$1 - Fe(1) -0.9482x + 13.0288y - 7.0431z = 7.1217 [N(1), 0.0711; N(2), -0.0691; N(1)_$1, 0.0731; O(1)_$1, -0.0751; Fe(1), 0.0681]
	2	N(2) - N(2)_$1 - O(1)_$1 - O(1) - Fe(1) 12.7411x - 0.0000y - 3.5417z = 5.4851 [N(2), -0.0404; N(2)_$1, 0.0404; O(1)_$1, -0.0380; O(1), 0.0380; Fe(1), 0.0000]
	3	N(1) - O(1) - N(1)_$1 - N(2)_$1 - Fe(1) 0.9482x + 13.0288y + 7.0431z = 11.5914 [N(1), 0.0731; O(1), -0.0751; N(1)_$1, 0.0711; N(2)_$1, -0.0691; Fe(1), 0.0681]

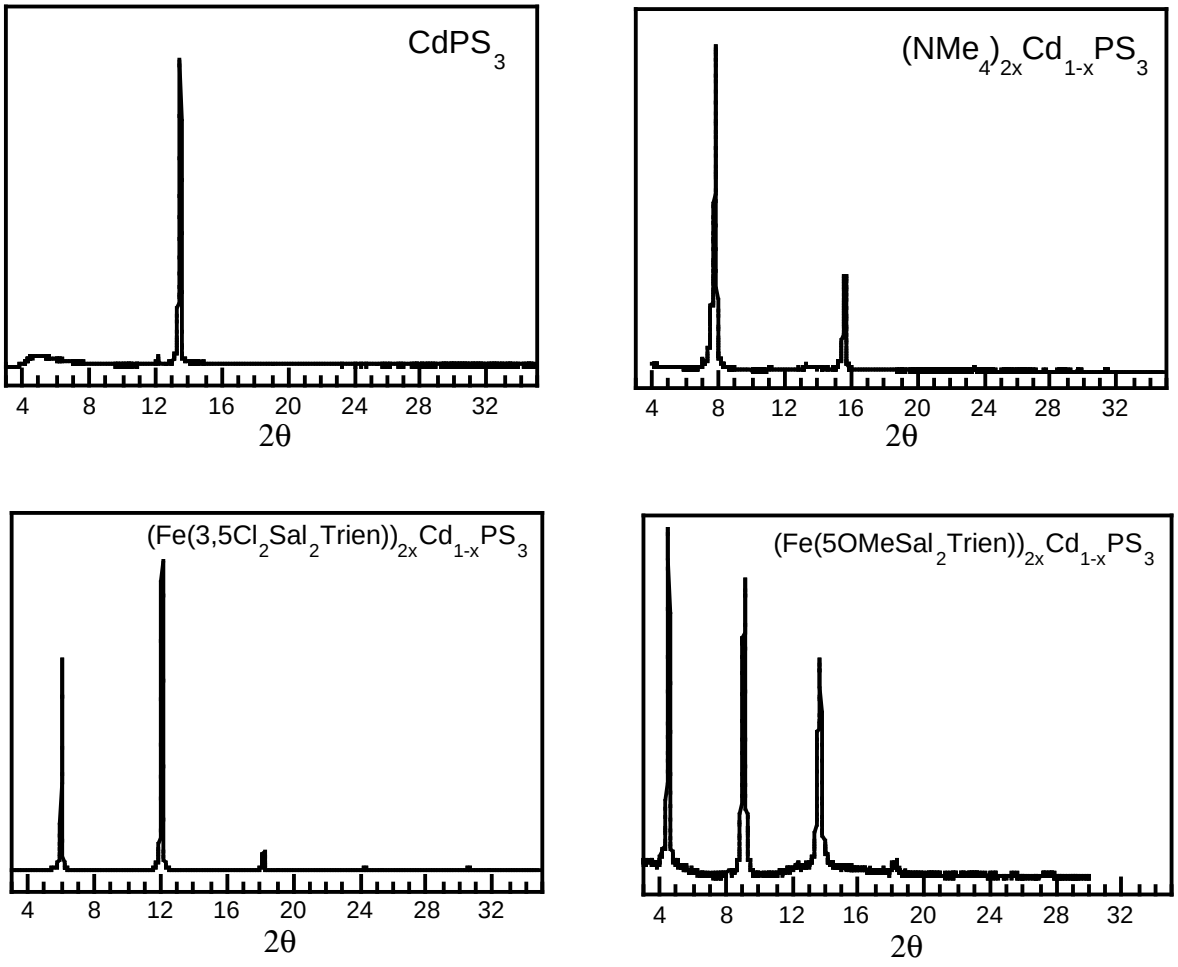

Figure S1 Powder X-Ray diffraction patterns of $CdPS_3$ and $CdPS_3$ intercalates.

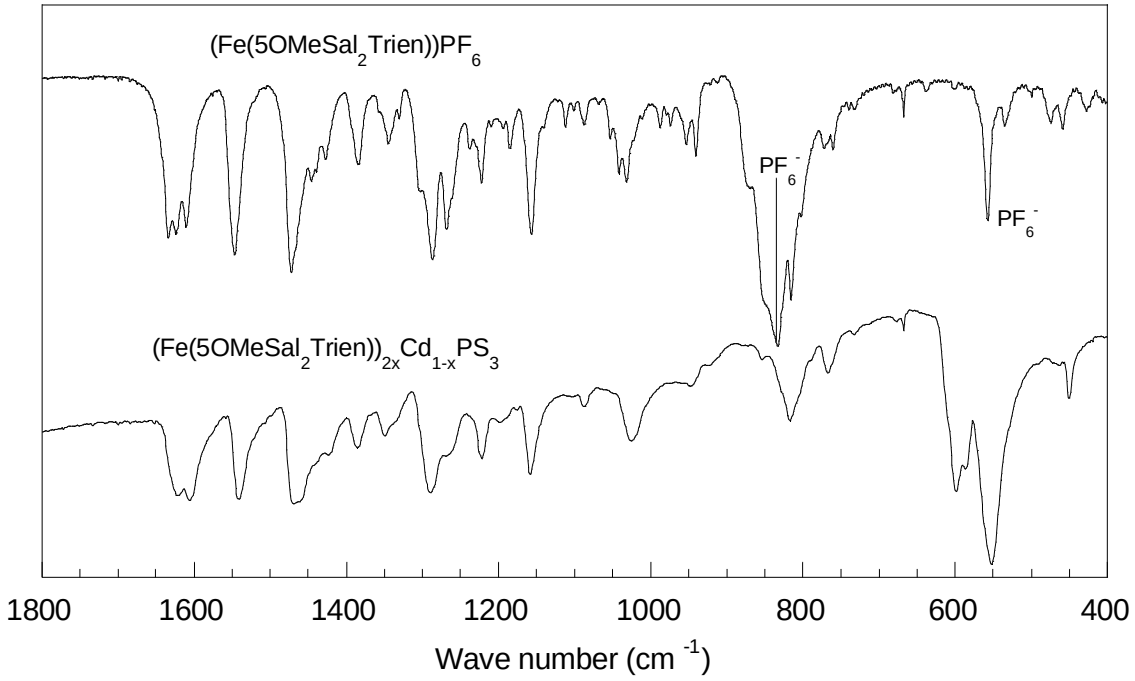

Figure S2 : Room temperature IR spectra of KBr pellets of $[Fe(5\text{-}OMe\text{-}Sal_2Trien)]_{2x}Cd_{1-x}PS_3$ (**10**) and $[Fe(5\text{-}OMe\text{-}Sal_2Trien)]PF_6$ (**5**).

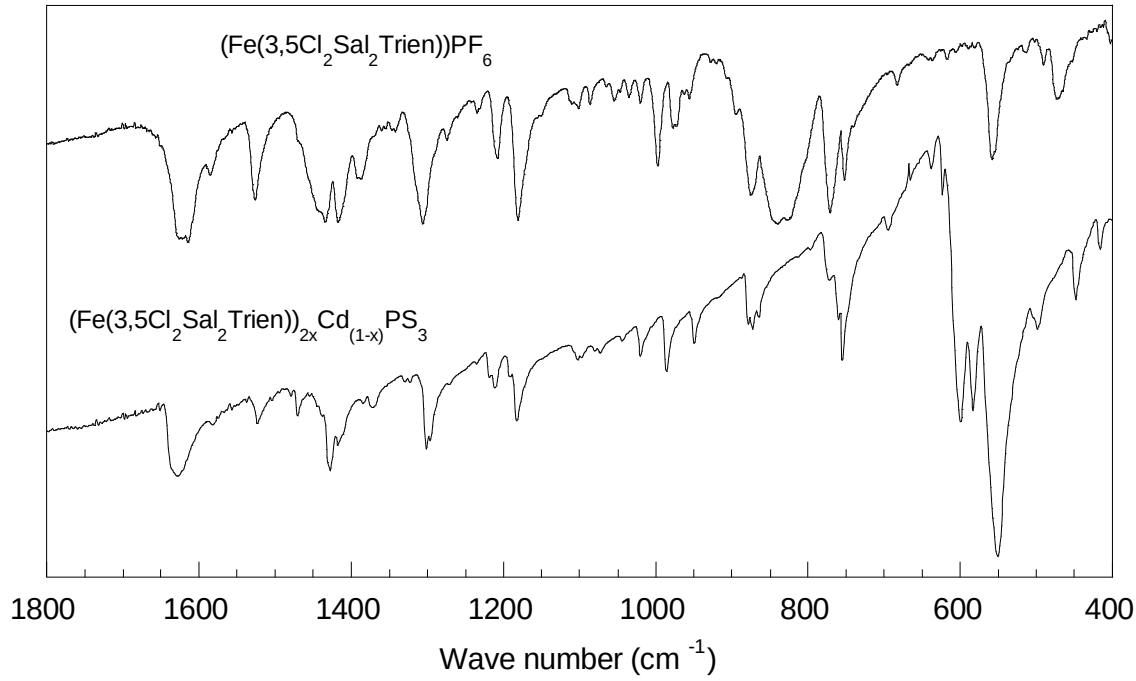

Figure S3 : Room temperature IR spectra of KBr pellets of $[Fe(3,5\text{-}Cl_2\text{-}Sal_2Trien)]_{2x}Cd_{1-x}PS_3$ (**9**) and $[Fe(3,5\text{-}Cl_2\text{-}Sal_2Trien)]PF_6$. **1**.