

Supplementary Materials: Effects of Internal and External Pressure on the $[\text{Fe}(\text{PM-PEA})_2(\text{NCS})_2]$ Spin-Crossover Compound (with PM-PEA = *N*-(2'-pyridylmethylene)-4-(phenylethynyl)aniline)

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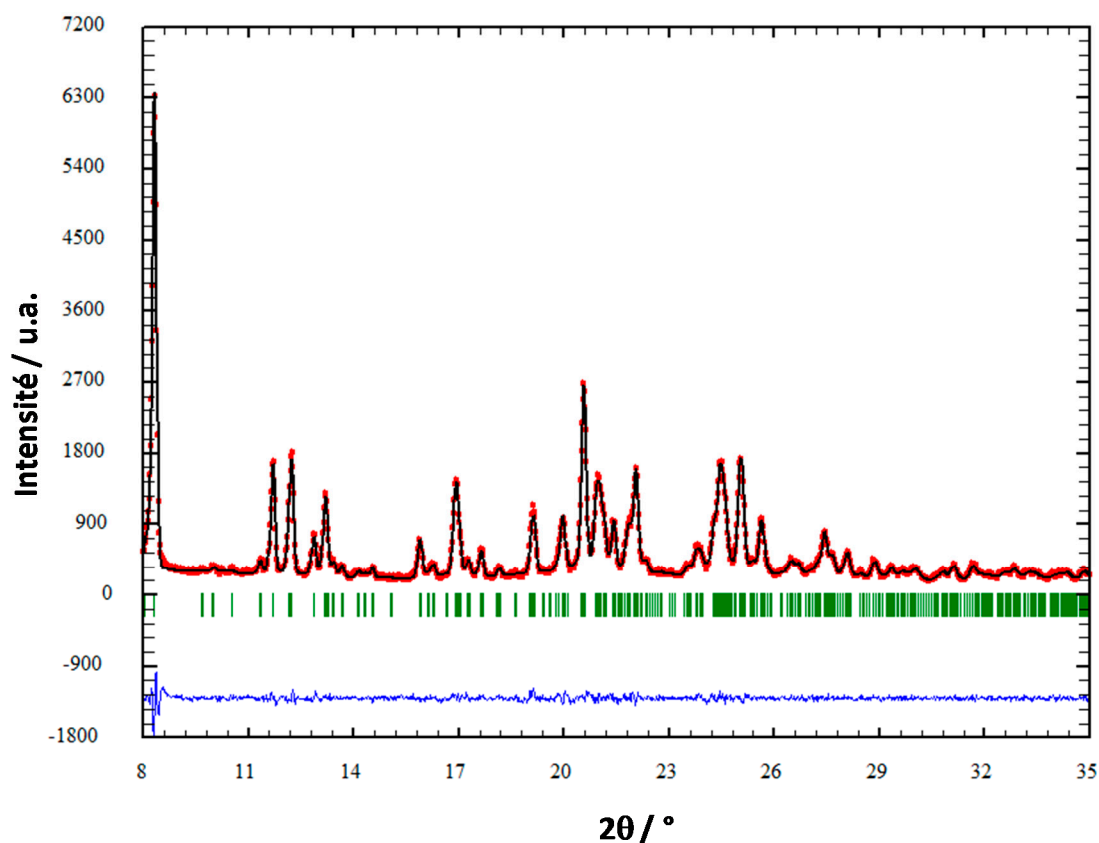


Figure S1. Le Bail refinement of the powder diffractogram of compound 1.

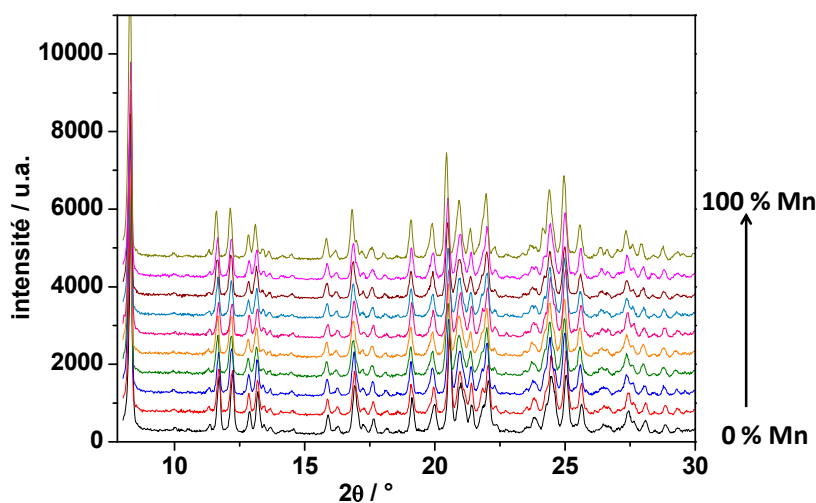


Figure S2. Powder diffractogram of compound 1–10.

Table S1. Unit-cell parameters extracted with the Le Bail refinements from powder X-ray diffraction.

Compounds	χ^2	a (Å)	b (Å)	c (Å)	β (°)
1: [Fe(PM-PEA) ₂ (NCS) ₂]	1.65	16.829	14.559	15.648	93.007
2: [Fe _{0.9} Mn _{0.1} (PM-PEA) ₂ (NCS) ₂]	1.74	16.812	14.550	15.652	92.974
3: [Fe _{0.85} Mn _{0.15} (PM-PEA) ₂ (NCS) ₂]	1.773	16.832	14.579	15.645	92.911
4: [Fe _{0.79} Mn _{0.21} (PM-PEA) ₂ (NCS) ₂]	1.98	16.822	14.561	15.634	93.025
5: [Fe _{0.73} Mn _{0.27} (PM-PEA) ₂ (NCS) ₂]	1.95	16.845	14.571	15.643	93.032
6: [Fe _{0.68} Mn _{0.32} (PM-PEA) ₂ (NCS) ₂]	1.89	16.856	14.574	15.654	93.005
7: [Fe _{0.56} Mn _{0.44} (PM-PEA) ₂ (NCS) ₂]	1.548	16.849	14.573	15.648	93.044
8: [Fe _{0.48} Mn _{0.52} (PM-PEA) ₂ (NCS) ₂]	1.597	16.855	14.560	15.633	93.067
9: [Fe _{0.36} Mn _{0.64} (PM-PEA) ₂ (NCS) ₂]	1.651	16.897	14.571	15.569	93.080
10: [Mn(PM-PEA) ₂ (NCS) ₂]	1.876	16.937	14.579	15.646	93.127