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Supporting information for article:

Crystal structure and magnetic properties of the layered hybrid organic-inorganic compounds $M_2(OH)_2(C_{14}H_8O_4)$ ($M = Mn, Fe$)

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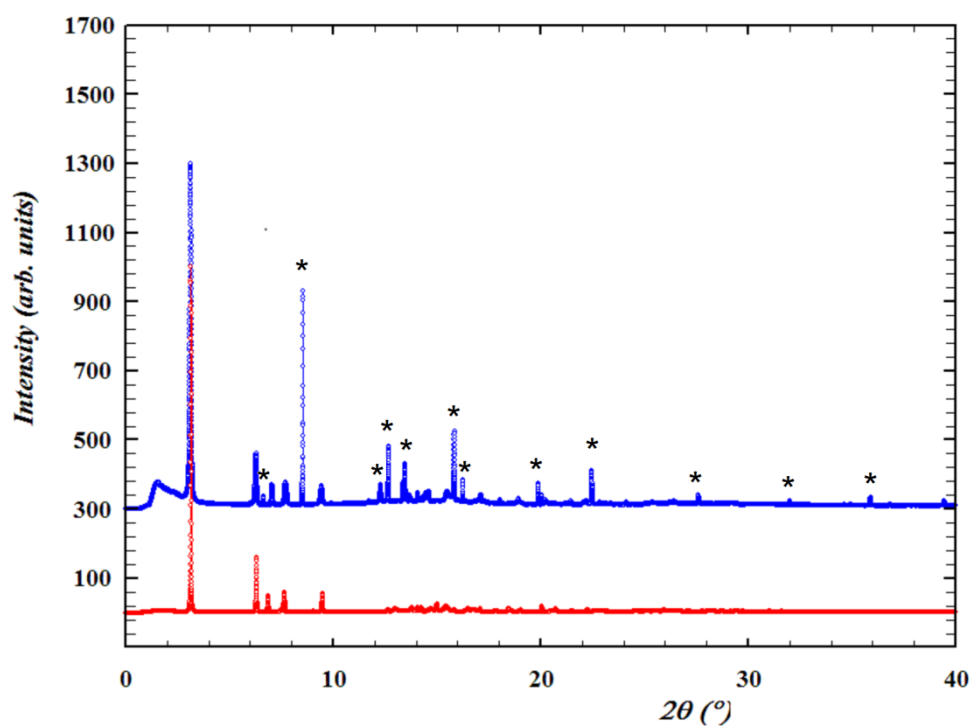


Figure S1 Raw synchrotron data for $M_2(OH)_2bpdc$, $M = Fe$ (blue) and Mn (red). Asterisk mark the impurity phase (unreacted 4,4'-biphenyldicarboxylic acid) in iron-based phase. $\lambda = 0.77752 \text{ \AA}$

Table S1 Fractional atomic coordinates for $Mn_2(OH)_2(bpdc)$

Code_Atom	Aom	x	y	z	B
M_1	C	-0.3753	0.610	0.953	3.3(2)
M_2	H	-0.3988	0.735	0.93	-
M_3	C	-0.2823	0.556	0.945	-
M_4	H	-0.2239	0.669	0.908	-
M_5	C	-0.2574	0.353	0.982	-
M_6	C	-0.3292	0.205	1.029	-

M_7	H	-0.3161	0.072	1.054	-
M_8	C	-0.4223	0.260	1.038	-
M_9	H	-0.4735	0.177	1.066	-
M_10	C	-0.4486	0.464	1.000	-
M_24	C	-0.1550	0.293	0.973	-
M_25	O	-0.1409	0.104	1.009	-
M_26	O	-0.0959	0.439	0.929	-
Mn1	Mn	0.000	0.000	0.000	1.5(2)
Mn2	Mn	0.000	0.500	0.500	2.2(2)
OH	O	0.0499(6)	0.172(2)	0.551 (10)	0.8(3)

Table S2 : M-O (Å) distances in M₂(OH)₂(bdc) (M = Mn, Fe, Co, Ni)

	Mn	Fe	Co	Ni	Cu
M1	Mn1	Fe1	Co1	Ni1	Cu1
- O _{COO}	2×2,278	2×2,157	2×2,105	2×2,106	2×2,021
- O _{OH}	4×2,173	4×2,128	4×2,182	4×2,041	2×1,847 ; 2×2,578
M2	Mn2	Fe2	Co2	Ni2	Cu2
- O _{COO}	4×2,235	4×2,189	4×2,204	4×2,209	2×2,037 ; 2×2,759
- O _{OH}	2×2,103	2×2,027	2×2,000	2×2,077	2×2,005

Tableau 1.3. Distances M – M (Å) et angles M – O – M (°) dans les composés M₂(OH)₂(bdc).

		Mn	Fe	Co	Ni	Cu
Distance	M1 – M2	3,677	3,582	3,550	3,545	3,553 ; 3,543
	M1 – M1 et M2 – M2	3,398	3,361	3,289	3,318	3,319
Angle	M1 – O _{OH} – M2	115,3	116,0	115,9	116,4	119,0
	M1 – O _{OH} – M1	102,7	102,5	98,0	104,6	108,5
	M2 – O _{COO} – M2	98,2	98,8	96,4	97,3	104,1

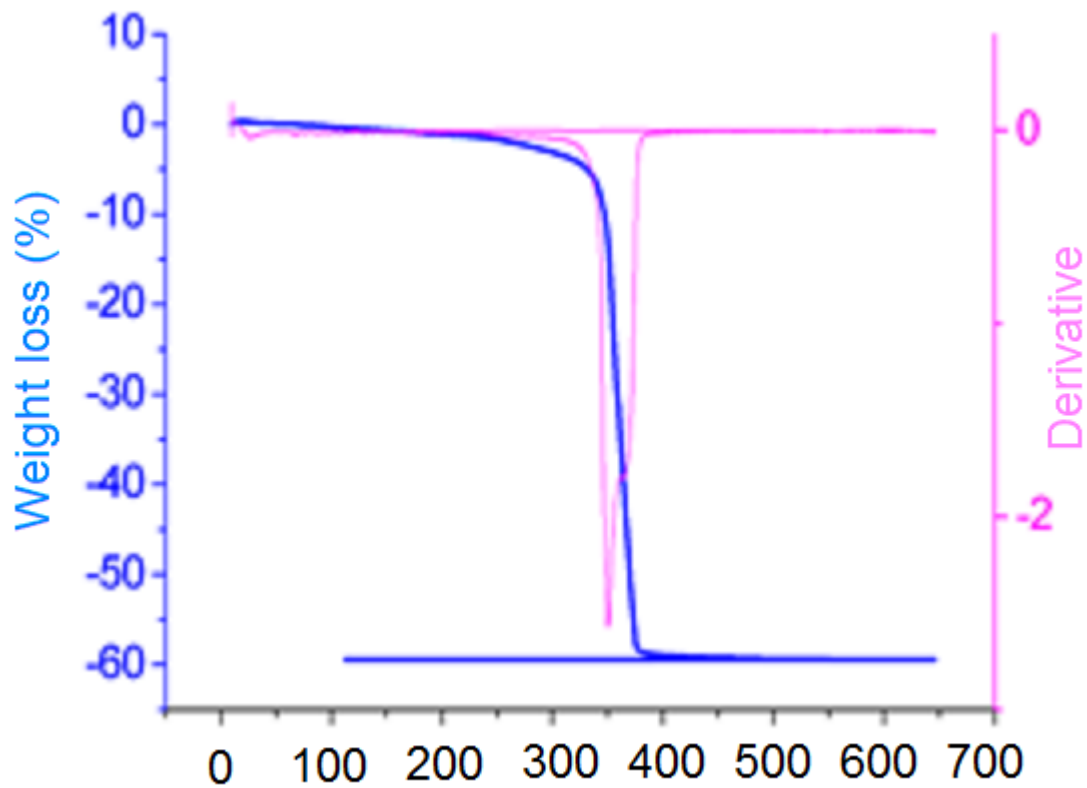


Figure S2 Thermogravimetric analysis of $\text{Mn}_2(\text{OH})_2(\text{bdc})$ recorded upon heating in air.