The first crystallographic and spectroscopic characterization of a 3*d*-metal borohydride: $Mn(BH_4)_2$

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Supporting Information

Table S1: Atomic Coordinates of $Mn(BH_4)_2$, s.g. $P3_112$, a=10.435(1), c=10.835(2) Å

Atom	**site**	***x***	***y***	***z***	B_{iso} [Å^2]
Mn1	6*c*	0.23130(50)	0.91807(72)	0.12532(40)	2.8(2)
Mn2	3*a*	0.56272(32)	2*x*	2/3	2.8
B1	6*c*	0.0403(34)	0.6990(30)	1.0056(58)	1.
H11	6*c*	-0.0824(33)	0.6582(70)	1.0014(67)	1.
H12	6*c*	0.0712(79)	0.6455(79)	0.9292(92)	1.
H13	6*c*	0.0685(66)	0.6689(49)	1.0980(89)	1.
H14	6*c*	0.1041(50)	0.8233(31)	0.9937(44)	1.
B2	3*b*	0.4708(31)	2*x*	1/6	1.
H21	6*c*	0.4285(44)	1.0140(63)	0.206(41)	1.
H22	6*c*	0.393(40)	0.8688(61)	0.0914(60)	1.
B3	3*a*	2*y*	0.1021(15)	0	1.
H31	6*c*	0.1323(30)	0.1145(36)	-0.0717(24)	1.
H32	6*c*	0.2766(30)	0.0642(23)	-0.0463(37)	1.
B4	3*a*	0.1329(17)	1-*x*	1/3	1.
H41	6*c*	0.0199(28)	0.8265(39)	0.3754(44)	1.
H42	6*c*	0.1250(54)	0.7875(42)	0.2588(29)	1.
B5	3*b*	0.7056(23)	1-*x*	5/6	1.
H51	6*c*	0.7531(36)	0.4149(28)	0.8590(98)	1.
H52	6*c*	0.716(11)	0.232(10)	0.9146(22)	1.

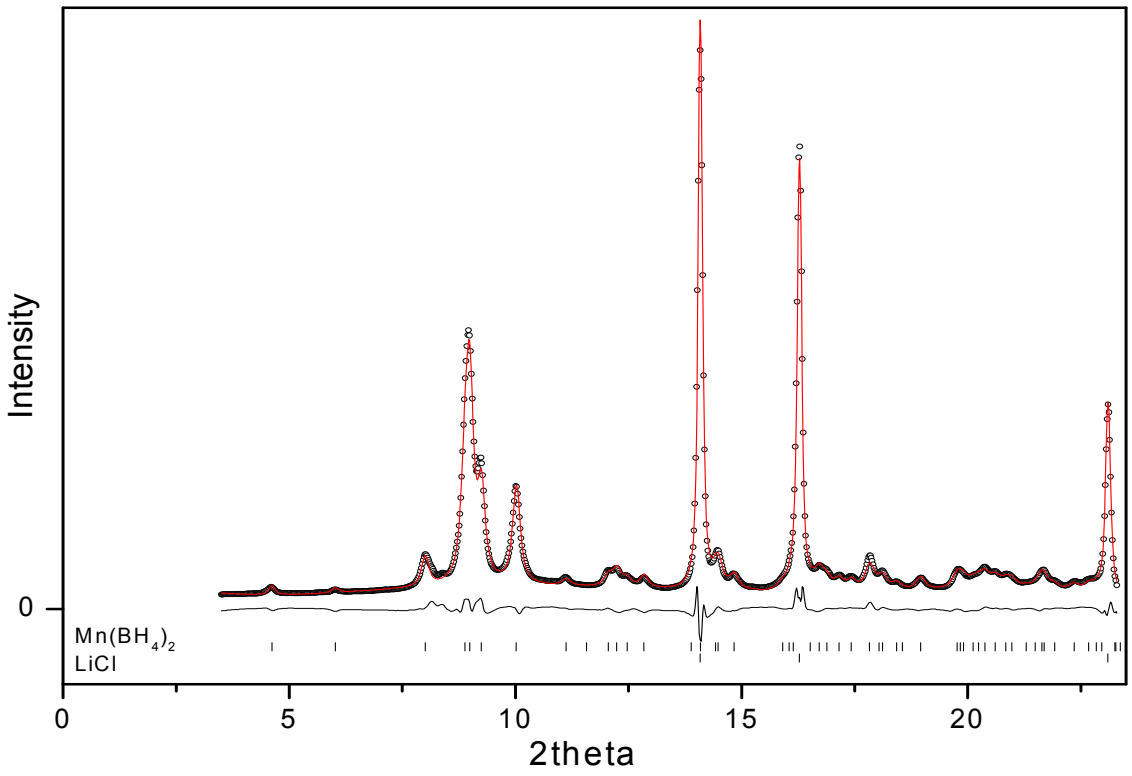

Figure S1. Rietveld plot of $Mn(BH_4)_2$ and the image-plate powder diffraction data measured at 295 K, using 0.72846 Å wavelength.

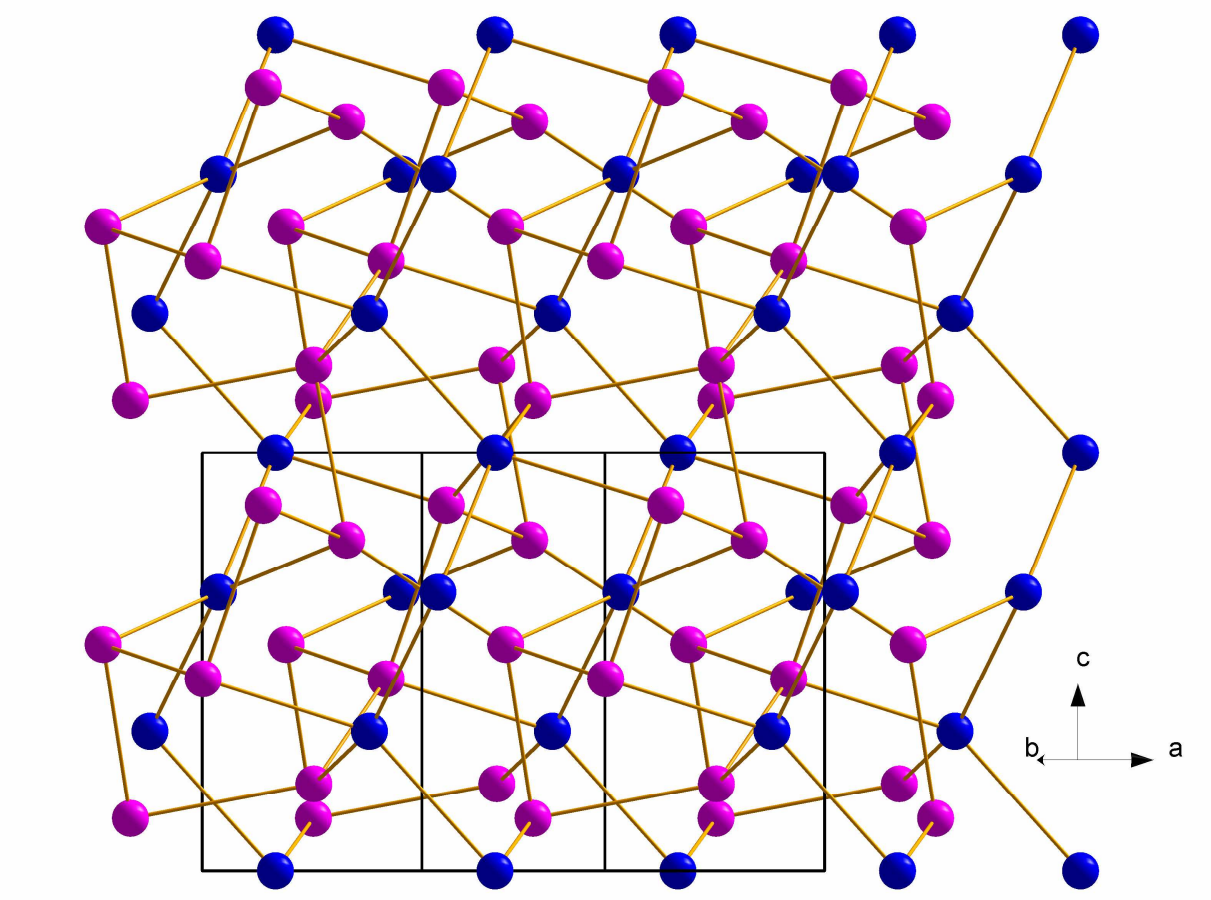

Figure S2. A novel tetrahedral framework topology in $Mn(BH_4)_2$. Four-connected Mn nodes are shown. Mn…Mn distances range from 4.71 to 4.86 Å.