Supplementary material

Structural studies of lithium zinc borohydride by neutron powder diffraction, Raman and NMR spectroscopy

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Table S1: **The refined crystal structure of $LiZn_2(^{11}BD_4)_5$ from PND data at 295K**

Atom	**Wyck.**	**x/*a***	**y/*b***	**z/*c***	***U* [Å^2]**
Zn1	8f	0	0.6440(10)	0.7665(11)	0.0377(6)
Zn2	8f	0	0.4252(12)	0.6300(16)	0.0377(6)
Li1	8f	0	0.138(6)	0.434(6)	0.0300(13)
B1	8f	0	0.2580(4)	0.3166(5)	0.0574(24)
D11	8f	0	0.1912(4)	0.3101(17)	0.0778(10)
D12	8f	0	0.2807(10)	0.3903(5)	0.0778(10)
D13	16g	0.1153(7)	0.2798(7)	0. 2804(7)	0.0778(10)
B2	8f	0	0.3513(4)	0.0903(5)	0.0574(24)
D21	8f	0	0.2971(5)	0.0442(8)	0.0778(10)
D22	8f	0	0.4090(5)	0.0505(9)	0.0778(10)
D23	16g	0.1136(7)	0.3488(10)	0.1355(5)	0.0778(10)
B3	8f	0	0.5320(4)	0.7016(4)	0.0574(24)
D31	8f	0	0.4746(5)	0.7421(9)	0.0778(10)
D32	8f	0	0.5264(14)	0.6238(5)	0.0778(10)
D33	16g	0.1145(7)	0.5662(5)	0.7223(9)	0.0778(10)
B4	16g	0.2284(8)	0.3825(4)	0.5882(4)	0.0574(24)
D41	16g	0.1551(14)	0.4234(6)	0.5415(7)	0.0778(10)
D42	16g	0.3368(10)	0.4186(7)	0.6142(11)	0.0778(10)
D43	16g	0.1591(14)	0.3629(10)	0.6520(6)	0.0778(10)
D44	16g	0.2550(19)	0.3297(5)	0.5424(8)	0.0778(10)

The space group is *Cmca* and unit cell dimensions are: a = 8.6031(13) Å, b = 17.8876(4) Å, c = 15.3598(3) Å, and Z = 8. Atomic coordinates and isotropic displacement factors for $LiZn_2(^{11}BD_4)_5$ are given above. The agreement factors are R_{wp} = 2.78 %, R_p = 2.22 %, and χ^2 = 1.56 (not corrected for background).

Table S2: **Selected interatomic distances (Å) and angles (º) in $LiZn_2(^{11}BD_4)_5$**

		Average:			
Zn1-D13	2x	1.833(18)		Zn-D	1.84
Zn1-D23	2x	1.799(16)			
Zn1-D33	2x	1.835(18)			
Zn2-D31		1.96(3)			
Zn2-D32		1.81(3)			
Zn2-D41	2x	1.91(2)			
Zn2-D43	2x	1.79(2)			
Zn1-B1		2.168(19)		Zn-B	2.20
Zn1-B2		2.201(19)			
Zn1-B3		2.238(19)			
Zn2-B3		2.20(2)			
Zn2-B4	2x	2.204(12)			
B1-Zn1-B2		123.9(7)	B-Zn-B		119.9
B1-Zn1-B3		117.5(7)			
B2-Zn1-B3		118.6(7)			
B4-Zn2-B4		126.2(9)			
B4-Zn2-B3	2x	116.5(9)			
Li1-D11		2.13(10)		Li-D	2.13
Li1-D12		2.64(11)			
Li1-D21		2.05(10)			
Li1-D22		1.98(10)			
Li1-D42	2x	1.88(7)			
Li1-D44	2x	2.22(4)			
Li1-B1		2.80(10)		Li-B	2.50
Li1-B2		2.41(9)			
Li1-B4	2x	2.39(2)			
B1-Li1-B2		125(3)			
B1-Li1-B4	2x	91(3)			
B2-Li1-B4	2x	99(3)			
B4-Li1-B4		156(4)			
Li1-B1-Zn1		176.0(17)	Li-B-Zn		169.8
Li1-B2-Zn1		173(3)			
Li1-B4-Zn2	2x	165(2)			

(**Table S2 continued)**

B1-D11		1.199(10)	D11-B1-D12		114.5(10)
B1-D12		1.203(12)	D11-B1-D13	2x	106.5(10)
B1-D13	2x	1.202(9)	D12-B1-D13	2x	109.0(9)
			D13-B1-B13		111.2(8)
B2-D21		1.201(13)	D21-B2-D22		113.2(8)
B2-D22		1.200(13)	D21-B2-D23	2x	108.1(8)
B2-D23	2x	1.200(8)	D22-B2-D23	2x	109.1(9)
			D23-B2-D23		109.1(9)
B3-D31		1.201(13)	D31-B3-D32		116.4(10)
B3-D32		1.199(10)	D31-B3-D33	2x	107.3(8)
B3-D33	2x	1.202(9)	D32-B3-D33	2x	107.8(10)
			D33-B3-D33		110.0(8)
B4-D41		1.203(13)	D41-B3-D42		106.1(9)
B4-D42		1.203(13)	D41-B3-D43		113.8(9)
B4-D43		1.200(13)	D41-B4-D44		103.2(9)
B4-D44		1.200(13)	D42-B4-D43		105.7(10)
			D42-B4-D44		118.0(10)
			D43-B3-D44		110.1(10)

Average:

B1-D	1.202	D-B1-D	109.5
B2-D	1.200	D-B2-D	109.4
B3-D	1.201	D-B3-D	109.5
B4-D	1.202	D-B4-D	109.5
B-D	1.201	D-B-D	109.5

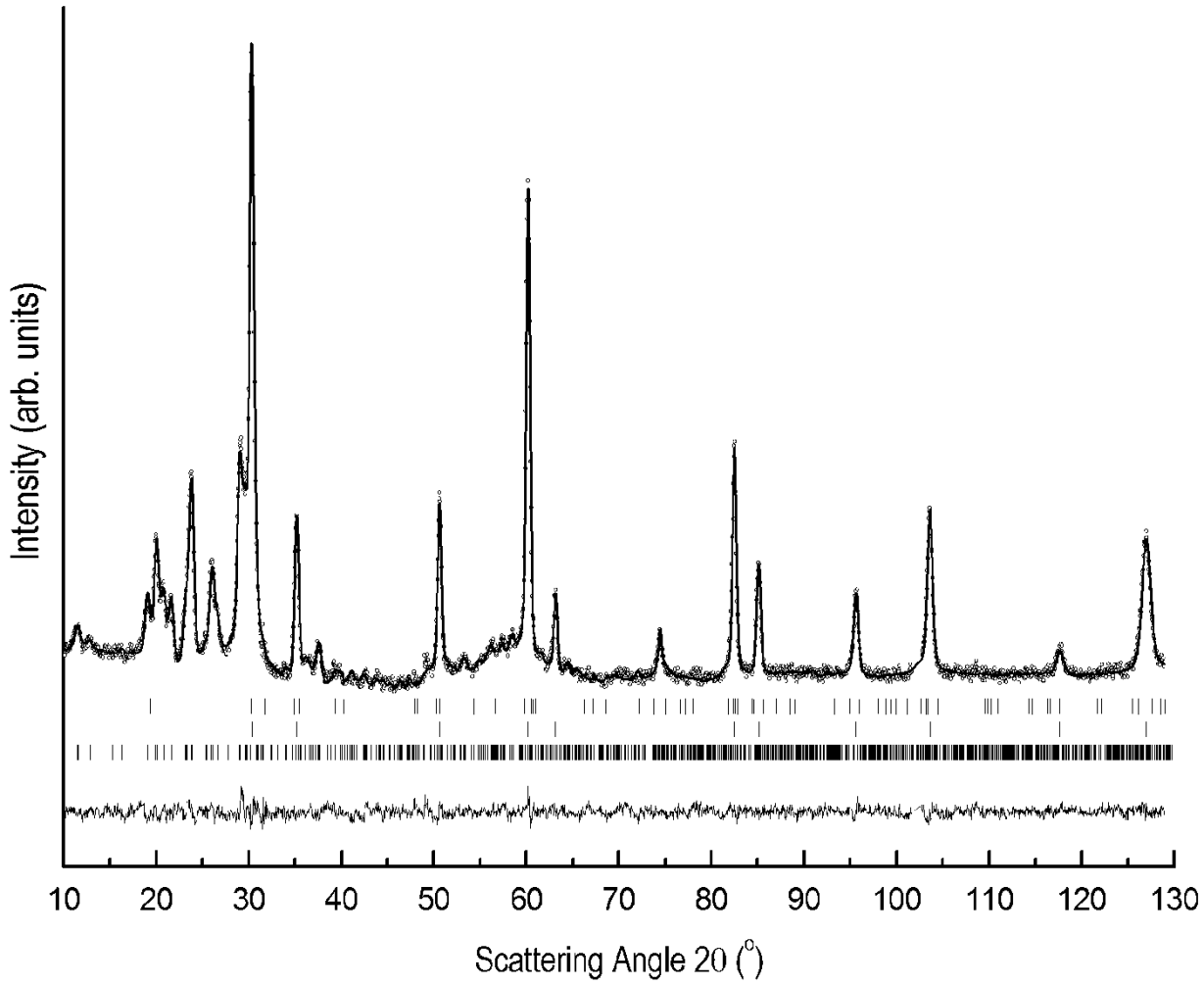

Fig. S1: Powder neutron diffraction pattern for $LiZn_2(^{11}BD_4)_5$ (sample A) measured at 295 K showing observed (circles), calculated (upper line) and difference (bottom line) plots. The position of the Bragg reflections are shown as tic marks for $LiZn_2(^{11}BD_4)_5$ (lower), LiCl (middle), and $ZnCl_2$ (upper) (λ = 1.55499 Å).