Supporting Information

Crystal Structures and Energy Storage Properties of Ammine Sodium Decahydro-*closo*-decaboranes ($Na_2B_{10}H_{10}\cdot nNH_3$, n = 1, 2)

Mathias Jørgensen,[a] Bjarne R. S. Hansen,[b] Young-Su Lee,[c] Young Whan Cho,[c] and Torben R. Jensen[*a]

[a]Interdisciplinary Nanoscience Center (iNANO) and Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark.

[b]Danish Technological Institute, Aarhus, Denmark

[c]Center for Energy Materials Research, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea

*Corresponding author

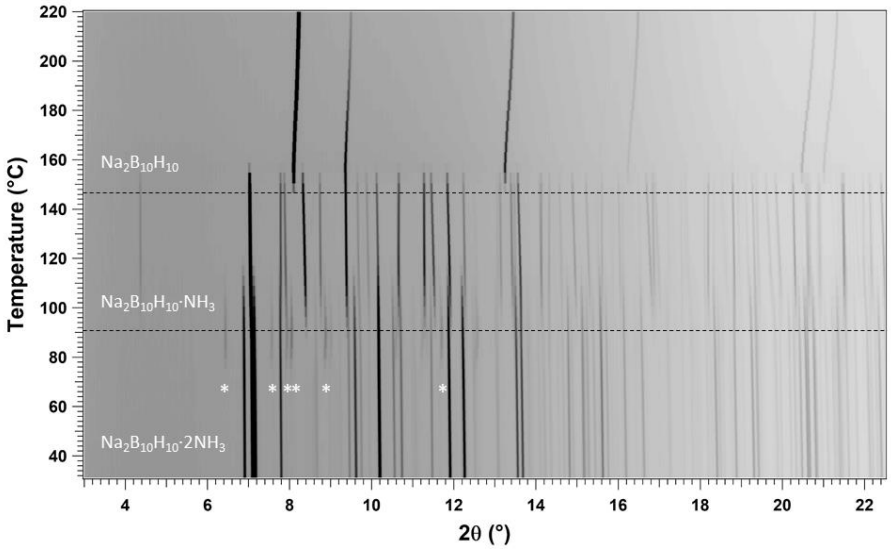

Figure S1: In situ PXD data of $Na_2B_{10}H_{10}\cdot 2NH_3$ heating from RT to 220 °C with a heating rate of 5 °C/min. λ = 0.82120 Å. Asterisks (*) mark the peaks from β-$Na_2B_{10}H_{10}\cdot NH_3$.

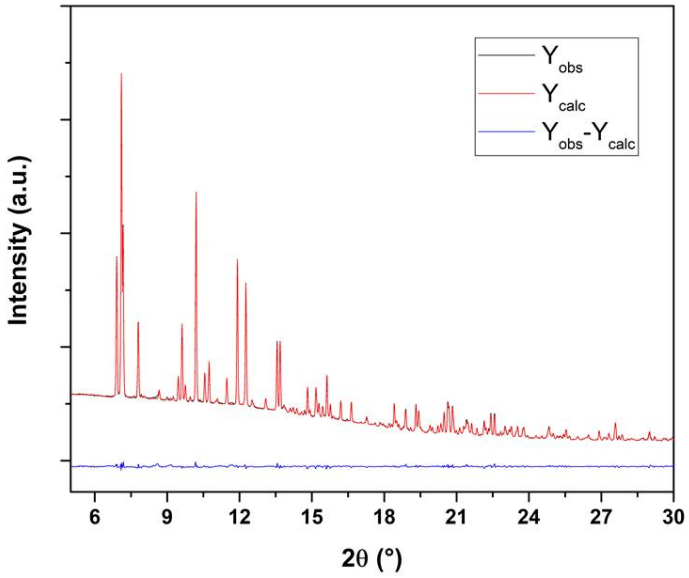

Figure S2: Simulated powder diffraction data of the modeled structure of $Na_2B_{10}H_{10}\cdot 2NH_3$ (Y_{calc}) compared with the observed PXD data (Y_{obs}). Agreement factors are: Rp = 6.69 %, Rwp = 5.28 % (both corrected for background) and R_{Bragg} = 3.59 %. λ = 0.82120 Å.

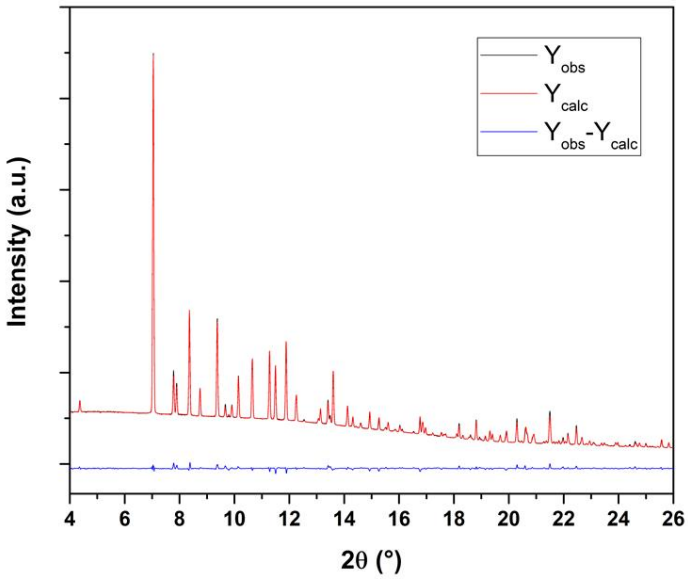

Figure S3: Simulated powder diffraction data of the modeled structure of $Na_2B_{10}H_{10}\cdot NH_3$ (Y_{calc}) compared with the observed PXD data (Y_{obs}). Agreement factors are: Rp = 10.3 %, Rwp = 8.76 % (both corrected for background) and R_{Bragg} = 5.41 %. λ = 0.82120 Å. T = 115 °C.

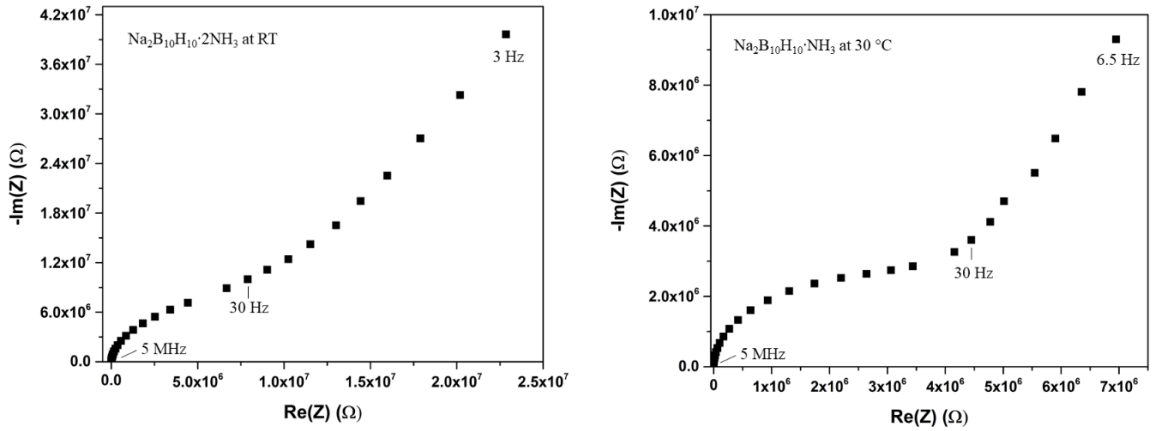

Figure S4: Impedance spectra **(**Nyquist plots) for: left: A 1.07 mm thick pellet of $Na_2B_{10}H_{10}\cdot 2NH_3$ measured at RT. Right: A 0.70 mm thick pellet of $Na_2B_{10}H_{10}\cdot NH_3$ measured at 30 °C. Tablet radius for both samples was 3.18 mm.

Table S1: Comparison between DFT and experimental cell parameters.

Chemical Formula	**$Na_2B_{10}H_{10}\cdot 2NH_3$**			**α-$Na_2B_{10}H_{10}\cdot NH_3$**		
	Exp.	Calc.	Deviation(%)	Exp.	Calc.	Deviation(%)
T [°C][a]	RT	0 K		115	0 K	
a [Å]	13.9492(1)	13.765	-1.3	13.9111(2)	13.778	-0.96
b [Å]	6.8925(7)	6.787	-1.5	7.0334(1)	6.898	-1.9
c [Å]	24.2240(2)	24.179	-0.19	21.6040(3)	21.318	-1.3
β [°]	94.0616(7)	93.16		94.4904(8)	95.10	
V [Å^3]	2323.19(12)	2256.0		2107.30(14)	2018.1	
Z	8	8		8	8	
V/Z	290.398(2)	281.0	-3.2	263.413(2)	252.3	-4.2

Table S2: Atomic position and displacement factors for the crystal structure of $Na_2B_{10}H_{10}\cdot 2NH_3$ (RT). The background hue delimits the different constituents.

Atom Label	**x**	**y**	**z**	**U_{iso} / Å^2**
N1	0.4474(3)	0.223(1)	0.5142(5)	0.077(1)
H11	0.4858(3)	0.209(1)	0.4892(5)	0.077(1)
H12	0.4317(3)	0.349(1)	0.4850(5)	0.077(1)
H13	0.4241(3)	0.114(1)	0.4821(5)	0.077(1)
N2	0.2836(3)	0.196(1)	0.0129(6)	0.077(1)
H21	0.3012(3)	0.267(1)	-0.0416(6)	0.077(1)
H22	0.2441(3)	0.248(1)	0.0123(6)	0.077(1)
H23	0.3037(3)	0.245(1)	0.0750(6)	0.077(1)

N3	0.2011(3)	0.302(1)	0.2424(6)	0.077(1)
H31	0.1818(3)	0.236(1)	0.1837(6)	0.077(1)
H32	0.1837(3)	0.244(1)	0.3006(6)	0.077(1)
H33	0.2408(3)	0.252(1)	0.2466(6)	0.077(1)
N4	-0.0406(4)	0.700(1)	0.2753(6)	0.077(1)
H41	-0.0553(4)	0.813(1)	0.2330(6)	0.077(1)
H42	-0.0587(4)	0.578(1)	0.2462(6)	0.077(1)
H43	0.0006(4)	0.690(1)	0.2647(6)	0.077(1)
B50	0.3508(2)	0.8850(5)	0.3209(3)	0.0249(9)
B51	0.3730(2)	0.8894(5)	0.1975(3)	0.0249(9)
B52	0.3443(2)	0.6486(5)	0.1726(3)	0.0249(9)
B53	0.3181(2)	0.6485(5)	0.2960(3)	0.0249(9)
B54	0.3075(2)	0.8375(5)	0.2196(3)	0.0249(9)
B55	0.4228(2)	0.8368(5)	0.3020(3)	0.0249(9)
B56	0.4185(2)	0.6724(5)	0.1962(3)	0.0249(9)
B57	0.3770(2)	0.4993(5)	0.2665(3)	0.0249(9)
B58	0.3838(2)	0.6629(5)	0.3689(3)	0.0249(9)
B59	0.4401(2)	0.5946(5)	0.3078(3)	0.0249(9)
H50	0.3408(2)	1.0036(5)	0.3701(3)	0.0249(9)
H51	0.3812(2)	1.0133(5)	0.1472(3)	0.0249(9)
H52	0.3284(2)	0.5740(5)	0.1052(3)	0.0249(9)
H53	0.2824(2)	0.5863(5)	0.3278(3)	0.0249(9)
H54	0.2676(2)	0.9124(5)	0.1911(3)	0.0249(9)
H55	0.4548(2)	0.9473(5)	0.3248(3)	0.0249(9)
H56	0.4455(2)	0.6566(5)	0.1332(3)	0.0249(9)
H57	0.3719(2)	0.3410(5)	0.2635(3)	0.0249(9)
H58	0.3835(2)	0.6291(5)	0.4454(3)	0.0249(9)
H59	0.4791(2)	0.5266(5)	0.3371(3)	0.0249(9)
B60	0.8795(2)	0.3096(5)	0.1305(3)	0.0249(9)
B61	0.8653(2)	0.5006(5)	0.0399(3)	0.0249(9)
B62	0.8233(2)	0.3364(5)	-0.0373(3)	0.0249(9)
B63	0.8344(2)	0.1446(5)	0.0576(3)	0.0249(9)
B64	0.8139(2)	0.3721(5)	0.0834(3)	0.0249(9)
B65	0.9325(2)	0.3688(5)	0.0498(3)	0.0249(9)
B66	0.8929(2)	0.3912(5)	-0.0686(3)	0.0249(9)
B67	0.8689(2)	0.1342(5)	-0.0548(3)	0.0249(9)
B68	0.9096(2)	0.1180(5)	0.0595(3)	0.0249(9)
B69	0.9372(2)	0.2053(5)	-0.0426(3)	0.0249(9)
H60	0.8898(2)	0.3177(5)	0.2088(3)	0.0249(9)

H61	0.8646(2)	0.6643(5)	0.0457(3)	0.0249(9)
H62	0.7885(2)	0.3596(5)	-0.0928(3)	0.0249(9)
H63	0.8100(2)	0.0237(5)	0.0817(3)	0.0249(9)
H64	0.7764(2)	0.4262(5)	0.1207(3)	0.0249(9)
H65	0.9706(2)	0.4464(5)	0.0786(3)	0.0249(9)
H66	0.8980(2)	0.4908(5)	-0.1325(3)	0.0249(9)
H67	0.8563(2)	0.0210(5)	-0.1074(3)	0.0249(9)
H68	0.9282(2)	-0.0097(5)	0.0951(3)	0.0249(9)
H69	0.9745(2)	0.1541(5)	-0.0763(3)	0.0249(9)
Na1	0.2924(2)	0.8512(8)	0.0062(3)	0.0640(6)
Na2	0.8026(2)	0.1438(8)	0.2552(3)	0.0640(6)
Na3	0.5458(2)	0.7416(6)	0.8174(4)	0.0640(6)
Na4	0.0501(2)	0.2742(7)	0.5519(4)	0.0640(6)

Table S2: Atomic position and displacement factors for the crystal structure of $Na_2B_{10}H_{10}{\cdot}NH_3$ (115 °C) in the conventional setting (Space group *C*2/*c*). The background hue delimits the different constituents.

Atom Label	**x**	**y**	**z**	**U_{iso} / Å^2**
N1	0.0675(2)	0.5416(7)	0.1176(4)	0.150(3)
H10	0.0901(2)	0.4982(7)	0.0596(4)	0.150(3)
H11	0.0976(2)	0.5177(7)	0.1766(4)	0.150(3)
H12	0.0321(2)	0.4472(7)	0.1231(4)	0.150(3)
B20	0.09925(9)	0.9100(4)	0.7813(2)	0.060(1)
B21	0.20623(9)	0.9341(4)	0.8816(2)	0.060(1)
B22	0.14223(9)	0.7588(4)	0.8710(2)	0.060(1)
B23	0.17479(9)	0.8489(4)	0.7735(2)	0.060(1)
B24	0.15215(9)	0.9164(4)	0.9743(2)	0.060(1)
B25	0.07689(9)	0.8984(4)	0.9038(2)	0.060(1)
B26	0.16304(9)	1.0847(4)	0.7914(2)	0.060(1)
B27	0.09093(9)	1.1291(4)	0.8471(2)	0.060(1)
B28	0.16656(9)	1.1463(4)	0.9182(2)	0.060(1)
B29	0.09925(9)	1.0958(4)	0.9683(2)	0.060(1)
H20	0.06159(9)	0.8710(4)	0.7170(2)	0.060(1)
H21	0.19782(9)	0.7658(4)	0.7105(2)	0.060(1)
H22	0.03011(9)	0.8164(4)	0.9188(2)	0.060(1)
H23	0.26045(9)	0.9179(4)	0.9041(2)	0.060(1)
H24	0.14061(9)	0.5912(4)	0.8852(2)	0.060(1)
H25	0.16910(9)	0.8481(4)	1.0505(2)	0.060(1)
H26	0.17946(9)	1.2013(4)	0.7361(2)	0.060(1)

H27	0.05591(9)	1.2475(4)	0.8132(2)	0.060(1)
H28	0.1968(9)	1.2791(4)	0.9482(2)	0.060(1)
H29	0.0750(9)	1.1744(4)	1.0309(2)	0.060(1)
Na1	0.2470(1)	0.5035(6)	0.8659(2)	0.1110(8)
Na2	0.5451(1)	0.6369(4)	0.6145(2)	0.1110(8)