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Structure and Hydrogen Storage Properties of the First Rare-earth Metal Borohydride Ammoniate: $Y(BH_4)_3 \cdot 4NH_3$

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Table S1 Experimental and crystallographic details for $Y(BH_4)_3 \cdot 4NH_3$

Chemical formula	$Y(BH_4)_3 \cdot 4NH_3$	
Formula weight	806.221 g/mol	
Crystal system	orthorhombic	
Space group	*Pc*2$_1$*n* (No. 33)	
Unit cell dimensions	a= 7.1151(1)Å	α= 90°
	b= 11.4192(2)Å	β= 90°
	c= 12.2710(2)Å	γ =90°
Z	4	
Density (calculated)	1.34269 g/cm^3	
Volume	997.02(2) Å^3	
2theta, deg	$2\theta_{min} = 3$, $2\theta_{max} = 83$	
Diffractometer	Mythen-II, AS	
Wavelength	1.3042 Å	
R_B	0.045	
R_{wp}	0.061	
Gof	1.747	

Table S2 Atomic coordinates of $Y(BH_4)_3 \cdot 4NH_3$

Atom	site	x	y	z
Y1	4a	0.45506(24)	0.71348(76)	0.89375(18)
B1	4a	0.6640(8)	0.5591(5)	0.8768(6)
H1a	4a	0.76771	0.48418	0.87533
H1b	4a	0.64170	0.58907	0.79005
H1c	4a	0.53096	0.52641	0.91678
H1d	4a	0.72314	0.63398	0.92645
B2	4a	0.1536(2)	0.6400(6)	0.8963(4)
H2a	4a	0.22632	0.59910	0.96880
H2b	4a	0.23643	0.61616	0.82097
H2c	4a	0.00447	0.60612	0.89452
H2d	4a	0.15113	0.73849	0.90568
B3	4a	0.1968(2)	0.3979(5)	0.9283(5)
H3a	4a	0.23011	0.30546	0.90192
H3b	4a	0.03961	0.40449	0.93990
H3c	4a	0.27831	0.41598	1.00559
H3d	4a	0.24258	0.46176	0.86316
N11	4a	0.7350(3)	0.3999(4)	0.6217(8)
H11a	4a	0.73503	0.39994	0.70246
H11b	4a	0.80062	0.47073	0.59490
H11c	4a	0.60385	0.39993	0.59488
N12	4a	0.5514(3)	0.1581(7)	0.9260(2)
H12a	4a	0.55143	0.07147	0.92602
H12b	4a	0.42024	0.18706	0.92602
H12c	4a	0.61704	0.18707	0.86015
N13	4a	0.9912(9)	0.1576(1)	0.8351(1)
H13a	4a	0.87830	0.10855	0.82361
H13b	4a	1.08887	0.11116	0.87305
H13c	4a	0.95773	0.22654	0.88001
N14	4a	0.2960(7)	0.3126(8)	0.1717(1)
H14a	4a	0.25135	0.26442	0.23351
H14b	4a	0.36122	0.38299	0.20001
H14c	4a	0.18747	0.33704	0.12665

Table S3 Calculated structural parameters of $Y(BH_4)_3 \cdot 4NH_3$ (Space group $Pc2_1n$, No. 33), (a = 7.4709 Å, b = 11.9902 Å, c = 12.8846 Å)

Atom	site	x	y	z
Y1	4a	0.45506	0.71348	0.89375
B1	4a	0.66400	0.55910	0.87680
H1a	4a	0.75196	0.46814	0.88111
H1b	4a	0.70850	0.60660	0.79491
H1c	4a	0.50199	0.52426	0.87876
H1d	4a	0.71380	0.61501	0.95672
B2	4a	0.15360	0.64000	0.89630
H2a	4a	0.26105	0.56773	0.92667
H2b	4a	0.19295	0.67394	0.80173
H2c	4a	-0.00078	0.60081	0.89005
H2d	4a	0.15229	0.72442	0.95655
B3	4a	0.19917	0.39785	0.92824
H3a	4a	0.19855	0.28603	0.92174
H3b	4a	0.03958	0.42375	0.95543
H3c	4a	0.30188	0.40683	0.99720
H3d	4a	0.24800	0.42853	0.83864
N11	4a	0.73500	0.39990	0.62170
H11a	4a	0.73503	0.39994	0.70246
H11b	4a	0.80062	0.47073	0.59490
H11c	4a	0.60385	0.39993	0.59488
N12	4a	0.55140	0.15810	-0.07400
H12a	4a	0.55143	0.07147	-0.07398
H12b	4a	0.42024	0.18706	-0.07398
H12c	4a	0.61704	0.18707	-0.13985
N13	4a	0.99120	0.15760	0.83510
H13a	4a	0.87830	0.10855	0.82361
H13b	4a	1.08887	0.11116	0.87305
H13c	4a	0.95773	0.22654	0.88001
N14	4a	0.29600	0.31260	0.17170
H14a	4a	0.25135	0.26442	0.23351
H14b	4a	0.36122	0.38299	0.20001
H14c	4a	0.18747	0.33704	0.12665

Table S4. Selected dihydrogen lengths (Å) in $Y(BH_4)_3 \cdot 4NH_3$

Bonds	**Length**
H1b…H14a	1.951
H1d…H12b	2.008
H3a…H13c	2.009
H3a…H12b	2.038
H3d…H14b	2.038
H3c…H14c	2.052
H3b…H11c	2.111
H2b…H12c	2.167
H2d…H11c	2.236
H2d…H13c	2.261
H2b…H13a	2.267
H3a…H13b	2.337
H1b…H13b	2.342
H2a…H12a	2.359
H3d…H14a	2.389

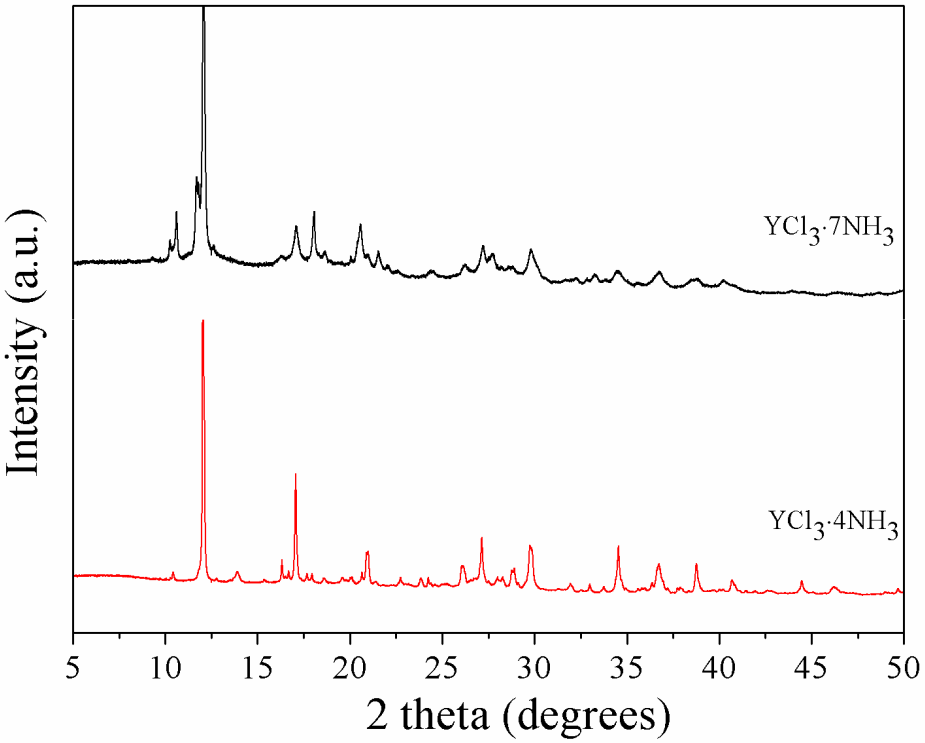

Fig. S1 High-resolution XRD pattern for $YCl_3 \cdot 7NH_3$ and $YCl_3 \cdot 4NH_3$.

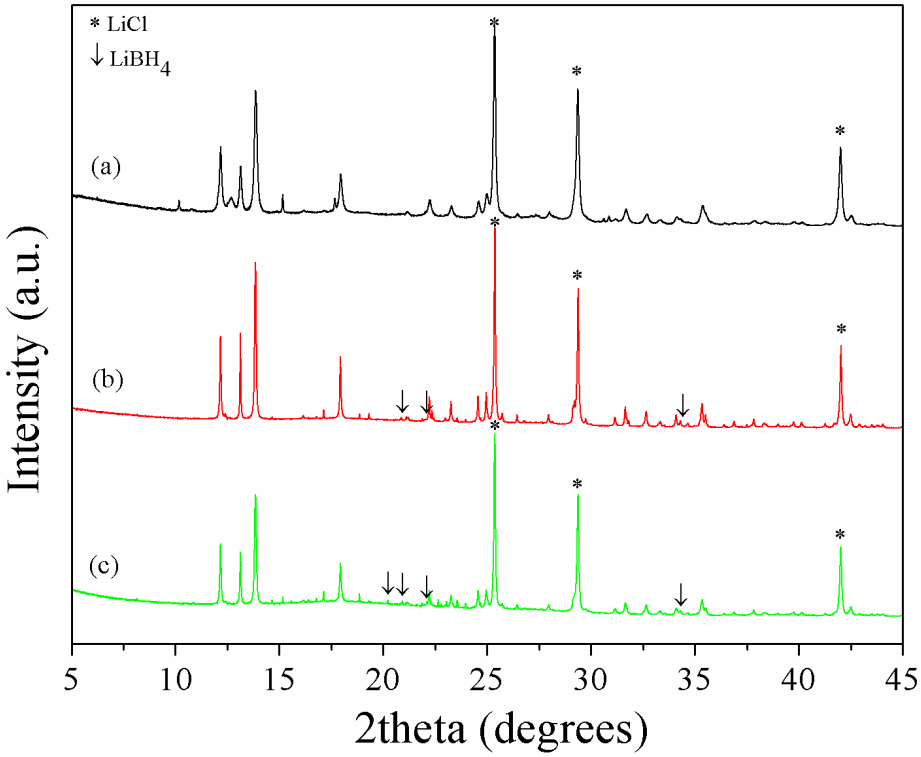

Fig. S2 High-resolution XRD profiles of milled-$YCl_3 \cdot 4NH_3/LiBH_4$ with mole rate of (a) 1:3, (b) 1:4 and (c) 1:5. LiCl and $LiBH_4$ peaks marked with star marks and arrow marks, respectively.