

Electronic Supporting Information
**Two novel derivatives of ammonia borane for hydrogen
storage: synthesis, structure, and hydrogen desorption
investigations**

**Leigang Li,^{a,b} Qinfen Gu,^c Ziwei Tang,^b Xiaowei Chen,^b Yingbin Tan,^b Qian Li,^{*a}
Xuebin Yu^{*b}**

^a*Shanghai Key Laboratory of Modern Metallurgy & Materials Processing, Shanghai University,
Shanghai, 200072, China.*

^b*Department of Materials Science, Fudan University, Shanghai, 200433, China.*

^c*Australian Synchrotron, 800 Blackburn Rd, Clayton, 3168, Australia.*

^a*Shanghai Key Laboratory of Modern Metallurgy & Materials Processing, Shanghai University,
Shanghai, 200072, China.*

Tel. & Fax: +86-21-56338065; E-mail: shuliqian@shu.edu.cn.

^b*Department of Materials Science, Fudan University, Shanghai, 200433, China.*

Tel.: +86-21-55664581; E-mail: yuxuebin@fudan.edu.cn;

Table S1 Atomic coordinates of 1,3-TMDAB

Atom	Wyck.	x/a	y/b	z/c
C10	4a	0.61938	0.29406	0.26431
C15	4a	0.72657	0.21651	0.23652
C16	4a	0.81714	0.33123	0.26460
N10	4a	0.52940	0.18532	0.23588
N15	4a	0.92181	0.25932	0.22770
B10	4a	0.41517	0.26542	0.24067
B15	4a	0.02064	0.37401	0.23593
H10	4a	0.53938	0.12836	0.11015
H20	4a	0.53387	0.09942	0.33613
H30	4a	0.61139	0.34142	0.40484
H40	4a	0.60903	0.39036	0.16650
H50	4a	0.41551	0.36700	0.12135
H60	4a	0.40271	0.32564	0.39165
H70	4a	0.34853	0.16693	0.20809
H15	4a	0.91889	0.20752	0.09745
H25	4a	0.93397	0.16853	0.31963
H35	4a	0.73061	0.16856	0.09518
H45	4a	0.73511	0.11866	0.33363
H55	4a	1.00753	0.47167	0.11379
H65	4a	0.02115	0.43785	0.38706
H75	4a	0.10103	0.29884	0.20970
H36	4a	0.81873	0.37522	0.40727
H46	4a	0.80955	0.43121	0.17131

Table S2 Kinetic modeling information of 1,2-TMDAB fitted by nucleation and growth model

Temperature	$[-\ln(1-\alpha)]^{2/3}=kt$		
	t (min)	k	r^2
100°C	≤10.50	0.0544	0.9984
110°C	≤6.50	0.1261	0.9970
120°C	≤7.06	0.1490	0.9922
130°C	≤5.66	0.2032	0.9928

Table S3 Kinetic modeling information of 1,2-TMDAB fitted by diffusion model

Temperature	$1 - \left(1 - \sqrt{\frac{t}{t_c}}\right)^3$		
	t (min)	t_c	r^2
100°C	>10.50	126.6	0.9566
110°C	>6.50	118.1	0.9817
120°C	>7.06	87.8	0.9471
130°C	>5.66	82.2	0.8745

Table S4 Kinetic modeling information of 1,3-TMDAB fitted by nucleation and growth model

Temperature	$[-\ln(1-\alpha)]^r = kt$			
	t (min)	r	k	R ²
100°C	≤60	3/2	0.0120	0.9988
110°C	≤13.69	1	0.0461	0.9973
120°C	≤10.36	1	0.0852	0.9747
130°C	≤10.97	1	0.1007	0.9993

Table S5 Kinetic modeling information of 1,3-TMDAB fitted by diffusion model

Temperature	$1 - \left(1 - \sqrt{\frac{t}{t_c}}\right)^3$		
	t (min)	t_c	r^2
100°C	--	--	--
110°C	>13.69	464.2	0.6823
120°C	>10.36	247.7	0.5286
130°C	>10.97	119.6	0.9917

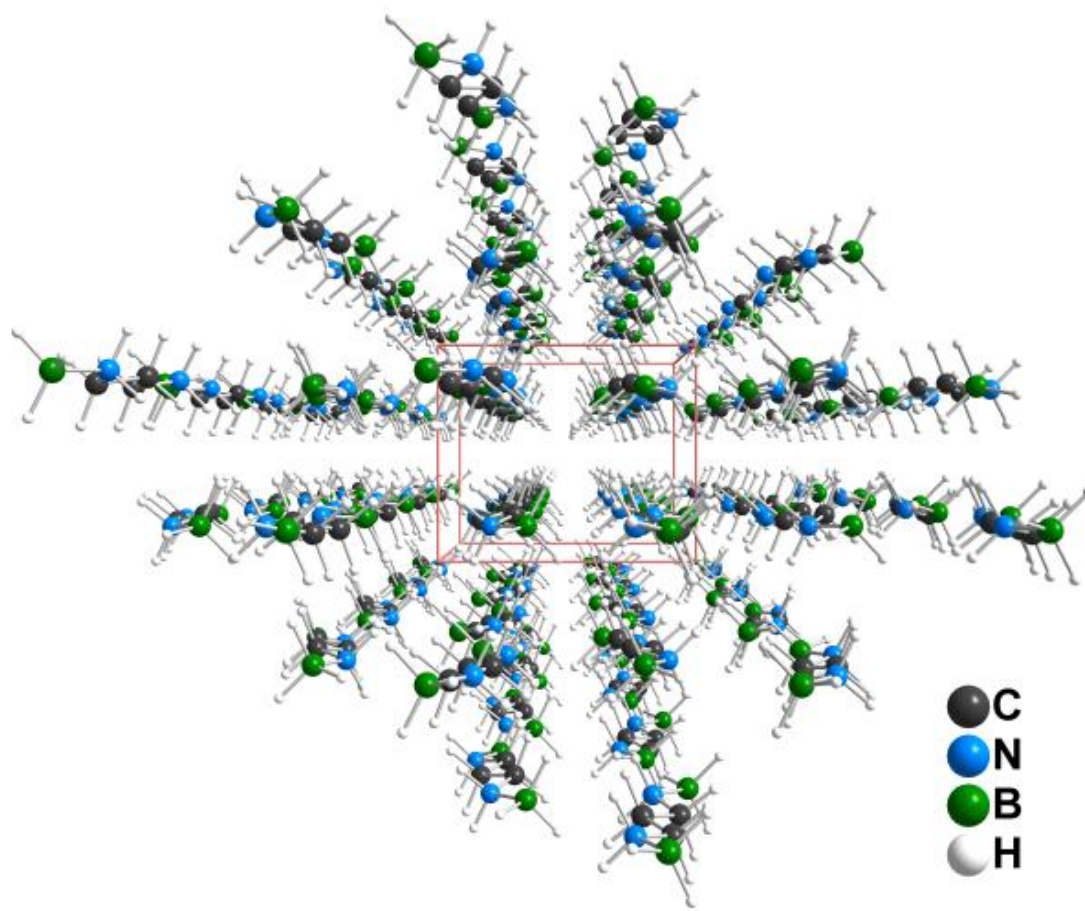


Fig. S1 3-D crystal structure of 1,3-TMDAB.

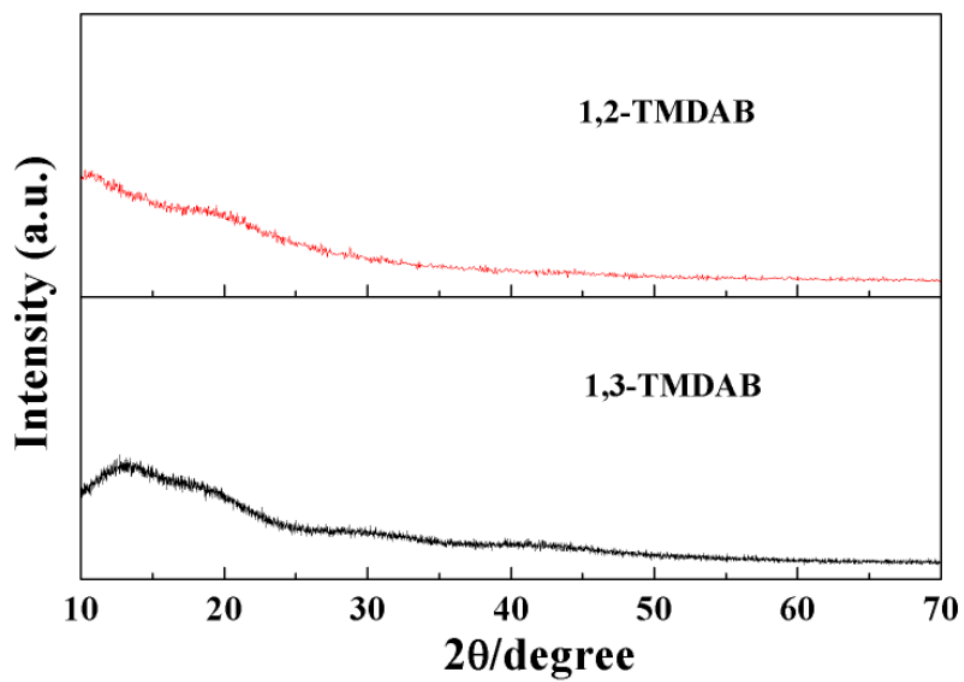


Fig. S2 XRD patterns of the decomposed products of 1,2-TMDAB and 1,3-TMDAB heated to 250 °C.