Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ELECTRONIC SUPLEMENTARY INFORMATION

"$M(BH_3NH_2BH_2NH_2BH_3)$ – the missing link in the mechanism of thermal decomposition of light alkali metal amidoboranes"

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Contents:

1. Synthesis of alkali metal M(B3N2) phases:

We used LiH, NaH (all 95%, Sigma Aldrich) and NH_3BH_3 (98%, JSC Aviabor) of the highest commercially available purity. We synthesized alkali metal M(B3N2) phases using dry THF as a solvent under argon atmosphere with no contact with atmospheric air, according to the reaction equations:

$$LiH + 3NH_3BH_3 \rightarrow Li[BH_3NH_2BH_2NH_2BH_3] + 1.5H_2\uparrow + NH_3\uparrow$$
$$NaH + 3NH_3BH_3 \rightarrow Na[BH_3NH_2BH_2NH_2BH_3] + 1.5H_2\uparrow + NH_3\uparrow$$

THF (99.9%, Sigma Aldrich) was firstly dried over yttrium borohydride or sodium hydride and then distilled. Reactions were performed in THF solution at room temperature with continuous stirring for 24h or in a disc mill in mechanosynthetic metod. The solid products were washed several times with fresh portions of THF and left to dry; they were analyzed without further purification. Samples were stored under argon atmosphere in Labmaster DP MBRAUN glovebox (O_2 < 1.0 ppm; H_2O < 1.0 ppm) at –35°C. All analyses were performed under inert atmosphere or in vacuum.)

The dry mechanochemical synthesis of Li(B3N2) and Na(B3N2) was carried out according to the method described by Evans. Milling was carried out using tungsten carbide disk milling vessel under argon atmosphere. We applied 3 steps of milling with 5 minutes breaks to avoid thermal decomposition of the milled product.

The synthesis consists of two stages: milling at room temperature and further heating of the byproduct at 75°C. In the first stage hydrogen is evolved while in the second stage, upon heating to 75°C ammonia is being desorbed along with formation of M(B3N2).

$$LiH + 3NH_3BH_3 \rightarrow LiNH_2BH_3{\cdot}NH_3BH_3 + NH_3BH_3 + H_2 \rightarrow Li[BH_3NH_2BH_2NH_2BH_3] + NH_3\uparrow + H_2\uparrow$$
$$NaH + 3NH_3BH_3 \rightarrow NaNH_2BH_3 + 2NH_3BH_3 + H_2\uparrow \rightarrow Na[BH_3NH_2BH_2NH_2BH_3] + NH_3\uparrow + H_2\uparrow$$

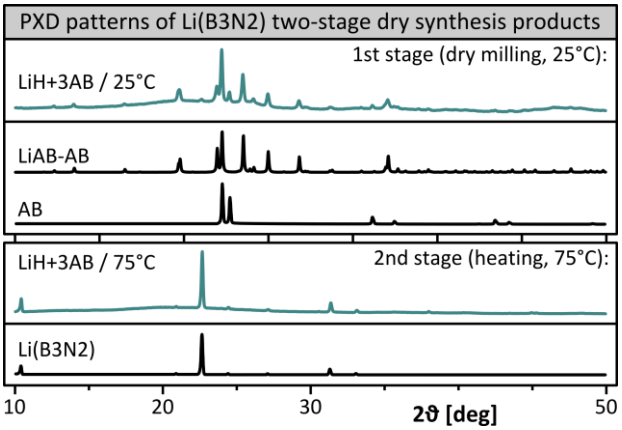

Fig. S1.1. PXD patterns of the products after each stage of Li(B3N2): dry milling (25°C) and heating (75°C).

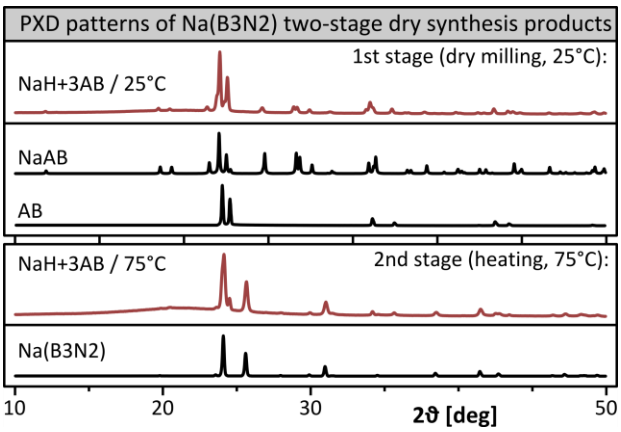

Fig. S1.2. PXD patterns of the products after each stage of Na(B3N2): dry milling (25°C) and heating (75°C).

2. Synthesis of alkali metal amidoboranes:

We used LiH, $LiNH_2$, NaH, $LiNH_2$ (all 95%, Sigma Aldrich) and NH_3BH_3 (98%, JSC Aviabor) of the highest commercially available purity.

We synthesized lithium and sodium amidoboranes via a dry mechanochemical way described in the literature, using tungsten carbide disk milling vessel together with a high energy mill from Testchem. All operations were carried out under argon atmosphere with no contact with atmospheric air, according to the reaction equations:

$LiNH_2 + NH_3BH_3 \rightarrow LiNH_2BH_3 + NH_3\uparrow$ 2 times per 3 minutes of milling

$NaH + NH_3BH_3 \rightarrow NaNH_2BH_3 + H_2\uparrow$ single 3 minutes milling

Milling was carried out with 5 minutes breaks to avoid thermal decomposition of the product during milling. Different milling regimes for different amidoboranes reflect optimization of the milling process due to stability differences of the products. Mechanochemical synthesis of potassium amidoborane was not performed due to high reactivity of potassium hydride with respect to ammonia borane (an uncontrolled solid-solid reaction commences already during mixing of the substrates).

We also synthesized sodium amidoboranes using dry THF as a solvent under argon atmosphere with no contact with atmospheric air, according to the reaction equations:

$NaH + NH_3BH_3 \rightarrow NaNH_2BH_3 + H_2\uparrow$

After the reaction the solvent was desorbed at room atmosphere.

3. Table of ^{11}B NMR @ THF-d_8 chemical shifts of alkali metal M(B3N2) phases and amidoboranes:

Table S3. Chemical shifts and J-coupling values observed in ^{11}B NMR spectra in deuterated THF solution (δ [ppm]) of alkali metal M(B3N2) [Li(B_3N_2), Na(B_3N_2)] and amidoboranes [LiAB, NaAB] at room temperature. Chemical shifts of fresh ammonia borane (AB) at RT are shown for comparison.

Band		amidoboranes		M(B3N2) phases	
	AB	LiAB	NaAB	Li(B3N2)	Na(B3N2)
BH_2 triplet	–	–	–	–8.360	–8.582
^1J (B,H)	–	–	–	103 Hz	99 Hz

Band		amidoboranes		M(B3N2) phases	
	AB	LiAB	NaAB	Li(B3N2)	Na(B3N2)
BH_3 quartet	–20.393	–20.051	–21.910	–22.562	–22.435
^1J (B,H)	95 Hz	86 Hz	86 Hz	90 Hz	91 Hz

4. Thermal decomposition of alkali M(B3N2) phases (TGA, PXD)

The thermal decomposition of Li(B3N2) and Na(B3N2) leads to formation of $LiBH_4$ and $NaBH_4$, respectively. For Li salt we observed emission of pure hydrogen around 140–160°C.

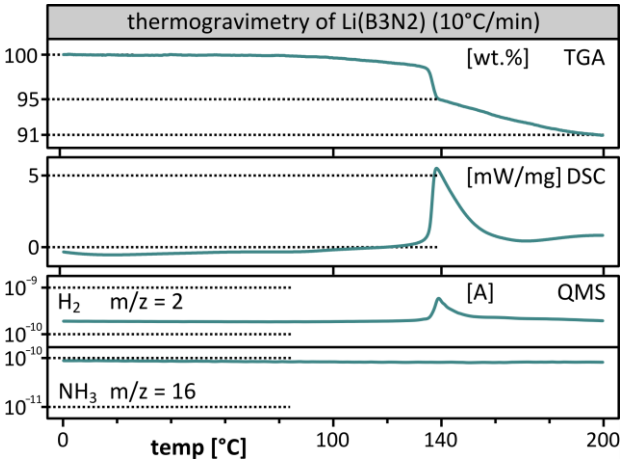

Fig. S4.1. TGA/DSC experiment with 10 K/min scanning rate of Li(B3N2) sample.

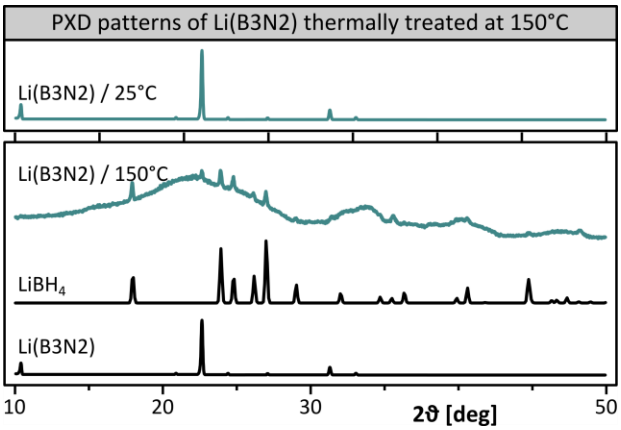

Fig. S4.2. PXD patterns of the product of thermal decomposition of Li(B3N2) sample.

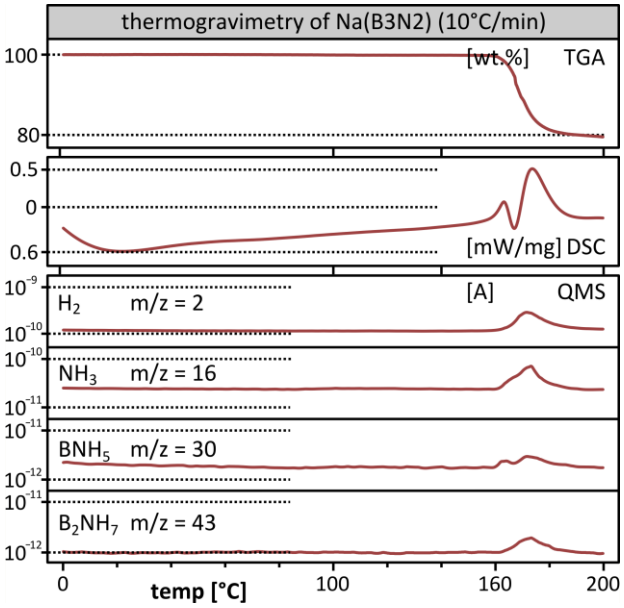

Fig. S4.3. TGA/DSC experiment with 10 K/min scanning rate of Na(B3N2) sample.

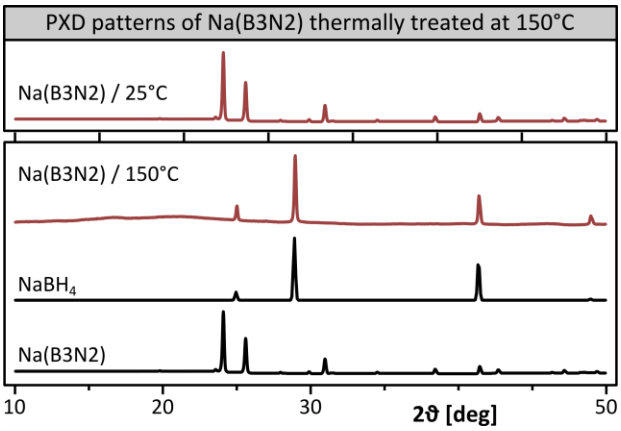

Fig. S4.4. PXD patterns of the product of thermal decomposition of Na(B3N2) sample.

5. Comparison of FTIR and Raman spectra of respective alkali M(B3N2) phases and amidoboranes:

There are characteristic differences observed in FTIR and Raman spectra of alkali metal M(B3N2) phases and amidoboranes. The NH and BH stretching regions have been highlighted. Magnification of the NH and BH stretching regions of FTIR and Raman spectra of alkali metal M(B3N2) phases and amidoboranes, is shown below.

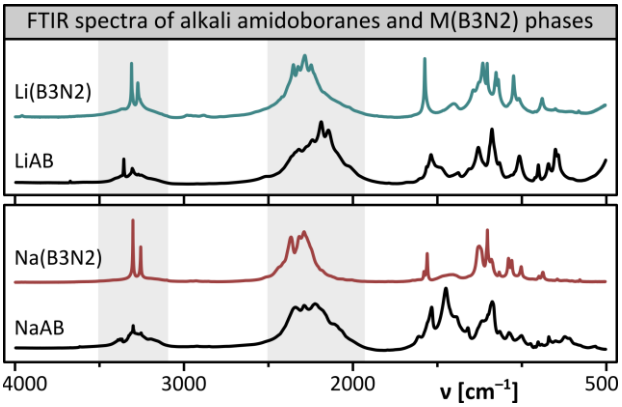

Fig. S5.1. Comparison of FTIR spectra of alkali metal M(B3N2) phases and respective amidoboranes.

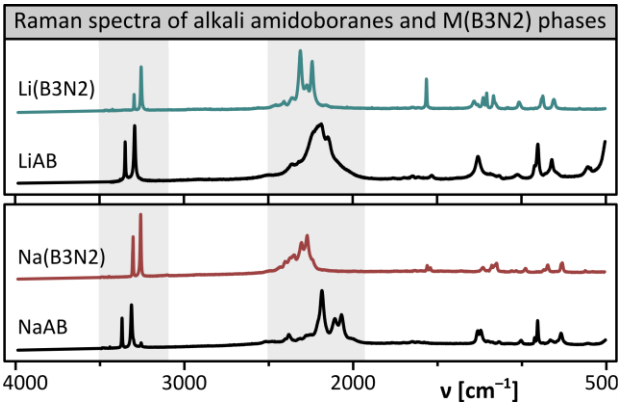

Fig. S5.2. Comparison of Raman spectra of alkali metal M(B3N2) phases and respective amidoboranes.

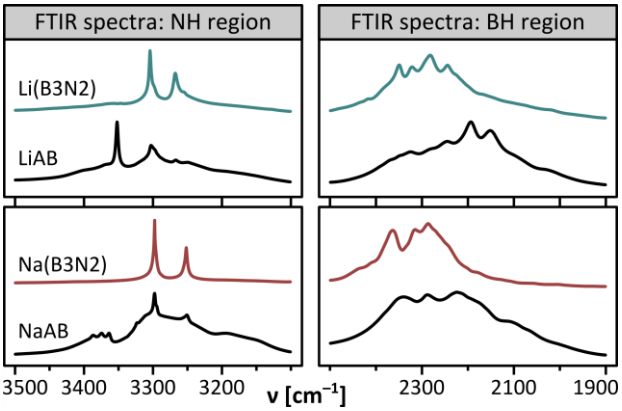

Fig. S5.3. Comparison of NH and BH stretching region of FTIR spectra of alkali metal M(B3N2) phases and respective amidoboranes.

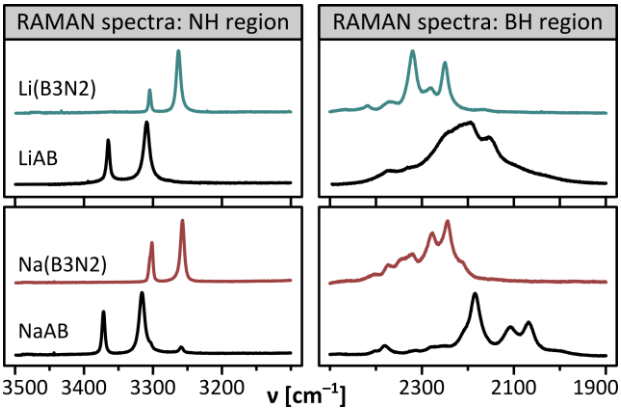

Fig. S5.4. Comparison of NH and BH stretching region of Raman spectra alkali metal M(B3N2) phases and respective amidoboranes.

6. Table of bands appearing in the FTIR spectra of alkali metal M(B3N2) phases and amidoboranes:

Table S6. Bands detected in IR absorption spectra (wavenumber [cm^{-1}]) of alkali metal M(B3N2) [Li(B3N2), Na(B3N2)] and amidoboranes (LiAB, NaAB) at room temperature. Absorption bands of fresh ammonia borane (AB) at RT are shown for comparison. (ν = stretching, δ = deformation: bending and torsional modes).

Band		amidoboranes		M(B3N2) phases	
	AB	LiAB	NaAB	Li(B3N2)	Na(B3N2)
ν(NH)			3393 vw		
			3380 vw		
		3370 sh	3369 vw		
		3359 m			
			3329 vw		
	3311 vs	3310 w	3303 m	3310 s	3302 vs
	3253 vs	3273 vw	3256 w	3273 m	3256 m
	3196 s	3251 vw	3200 vw		
		3185 sh			
ν(BH)				2350 vs	2364 s
	2347 vs	2326 m	2340 s	2322 s	2315 s
	2289 s	2280 sh	2289 s	2282 vs	2286 vs
		2245 s	2224 s	2245 s	
		2194 vs			
	2118 m	2152 s	2120 sh		
		2035 sh	2065 sh		
δ(NH)	1611 m	1605 sh	1608 w		
		1570 w		1571 vs	1576 w
		1544 m	1532 s		1556 m
		1495 sh			
δ(BH)		1315 sh	1317 m		
		1261 s	1260 sh	1283 m	1248 m
			1232 m	1226 s	
			1198 vs	1201 s	1199 vs
		1180 vs	1173 s		1175 m
	1163 vs	1165 sh		1148 s	
		1135 m	1129 w	1135 m	1129 vw
	1067 s	1065 sh	1074 w		1074 m
				1044 m	1055 m
		1016m	999 w	1013 w	999 w
ν(BN)		920 vw	922 vw	916 w	893 vw
		902 w	901 w		
and			880 vw	874 vw	870 w
other		842 w	837 w		
		800 m	797 w	799 vw	785 vw
		784 m	742 w		

7. Table of bands appearing in the Raman spectra of alkali M(B3N2) phases and amidoboranes:

Table S7. Bands detected in Raman scattering spectra (wavenumber [cm^{-1}]) of alkali metal M(B3N2) [Li(B3N2), Na(B3N2)] and amidoboranes (LiAB, NaAB) at room temperature. Absorption bands of fresh ammonia borane (AB) at RT are shown for comparison. (ν = stretching, δ = deformation: bending and torsional modes).

Band		amidoboranes		M(B3N2) phases	
	AB	LiAB	NaAB	Li(B3N2)	Na(B3N2)
ν(NH)	3314 m 3253 vs 3177 m	3361 s 3303 vs	3372 m 3314 s 3258 w	3314 m 3272 s	3265 vs 3221 s
ν(BH)	2378 vs 2284 vs	2368 w 2327 sh 2317 sh 2191 vs 2153 s	2376 w 2307 vw 2183 s 2103 m 2069 m 1987 sh	2418 vw 2370 w 2320 vs 2282 m 2250 s 2166 vw	2403 w 2373 w 2322 m 2275 s 2243 s 2214 sh
δ(NH)	1598 m 1583 m	1650 vw 1613 vw 1524 wv	1646 vw 1620vw 1563 vw	1567 m	1539 w 1519 vw
δ(BH)	1190 sh 1168 m 1069 vw	1152 m 1122 vw 1021 vw	1260 w 1242 w 1202 vw 1172 vw 1130 vw 1001 vw	1281 w 1259 vw 1226 w 1206 m 1166 w 1010 w	1212 w 1162 w 1132 w 1047 vw 1019 vw
ν(BN) and other	800 w 785 m 729w	919 m 901 s 818 m 603 w 584 w	922 w 904 m 829 vw 764 w 594 vw	895 vw 873 w 806 w	856 vw 835 w 749 w 614 vw

8. Relative thermal stability of alkali metal M(B3N2) phases and respective amidoboranes

We noticed significant differences between in thermal stability of alkali amidoborane and respective M(B3N2) phases at room temperature.

LiAB, NaAB and $NaLi(AB)_2$ each undergo decomposition leading to formation of M(B3N2) phases at room temperature. Over some period of time significantly strong reflections from Li(B3N2) or Na(B3N2) phases can be detected in the samples of LiAB, NaAB and $NaLi(AB)_2$. The resulting Li(B3N2) and Na(B3N2) are stable at room temperature.

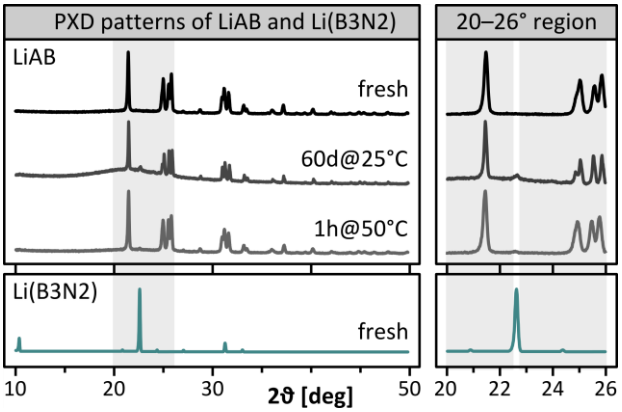

Fig. S8.1. Relative stability of LiAB and Li(B3N2). PXD patterns of fresh, aged and thermally treated samples of LiAB (top) compared with PXD pattern of Li(B3N2) (bottom). Region of 20–26° is marked grey and magnified in the section on the section on the right hand side.

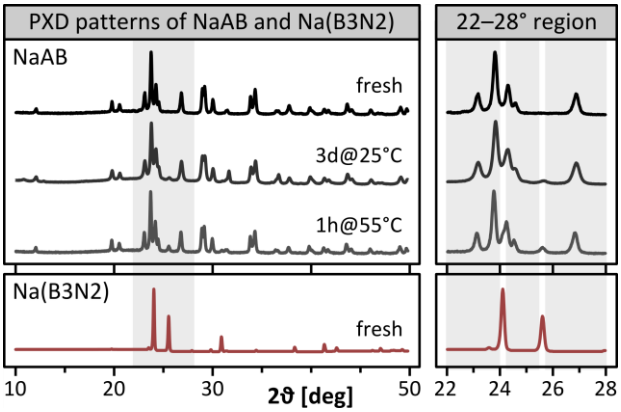

Fig. S8.2. Relative stability of NaAB and Na(B3N2). PXD patterns of fresh, aged and thermally treated samples of NaAB (top) compared with PXD pattern of Na(B3N2) (bottom). Region of 22–28° is marked grey and magnified in the section on the section on the right hand side.

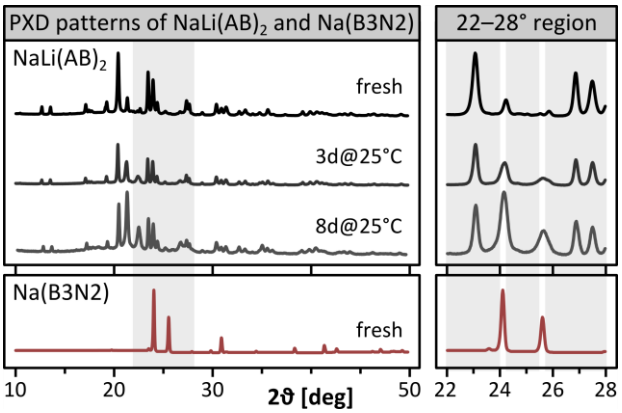

Fig. S8.3. Relative stability of $NaLi(AB)_2$ and Na(B3N2). PXD patterns of fresh, aged and thermally treated samples of $NaLi(AB)_2$ (top) compared with XRD pattern of Na(B3N2) (bottom). Region of 22–28° is marked grey and magnified in the section on the section on the right hand side.

9. Alkali metal M(B3N2) phases overlooked in the previous studies

In some previous papers on alkali metal amidoboranes several authors have presented PXD patterns indicating the presence of not only MAB phases but also of some (then unknown) phases. In the view of our results we can now assign most of these reflections to alkali metal M(B3N2) phases.

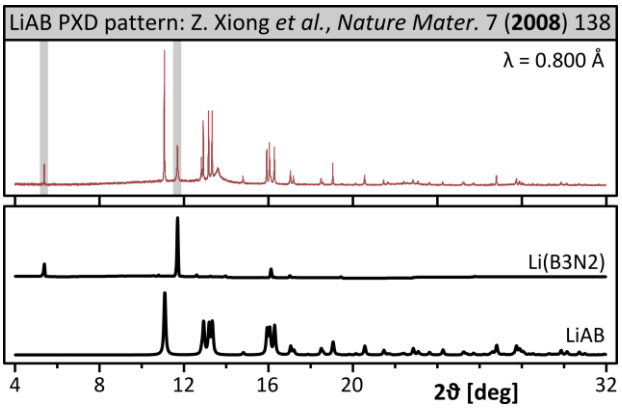

Fig. S9.1. PXD powder pattern of LiAB presented by Z. Xiong *et al* in 2008 in Nature Materials (top). Signals representing Li(B3N2) are marked with grey stripes (top). For comparison PXD patterns of LiAB and Li(B3N2) are shown (bottom).

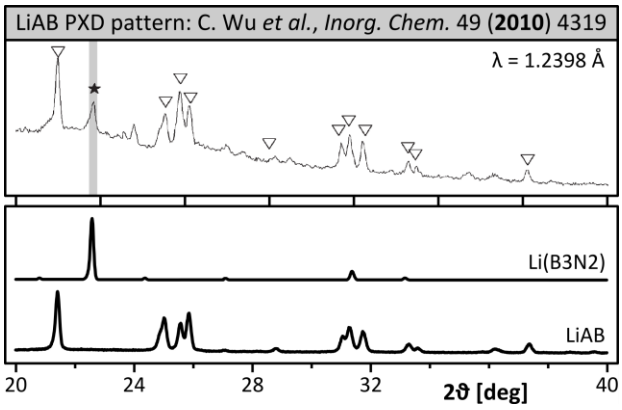

Fig. S9.2. PXD powder pattern of LiAB presented by C. Wu *et al* in 2010 in Inorganic Chemistry (top). Signals representing Li(B3N2) are marked with grey stripes (top). For comparison PXD patterns of LiAB and Li(B3N2) are shown (bottom).

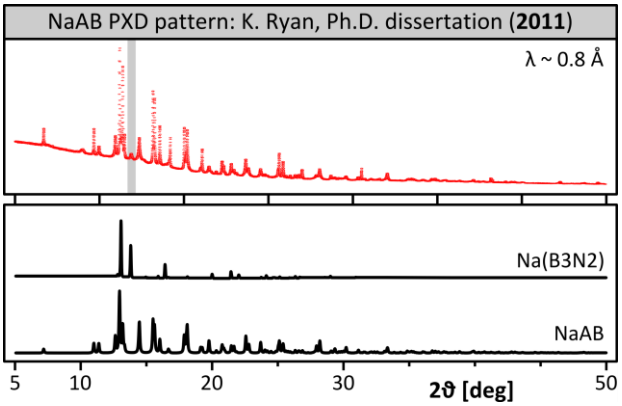

Fig. S9.3. PXD powder pattern of NaAB presented by K. Ryan in 2011 in her Ph.D. dissertation (top). Signals representing Na(B3N2) are marked with grey stripes (top). For comparison PXD patterns of NaAB and Na(B3N2) are shown (bottom).

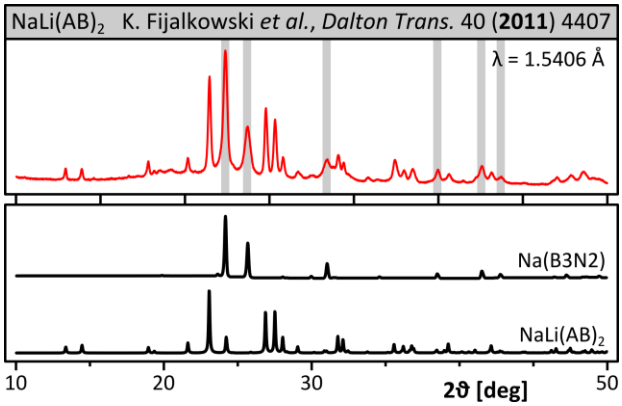

Fig. S9.4. PXD powder pattern of $NaLi(AB)_2$ presented by K. J. Fijalkowski *et al* in 2011 in Dalton Transactions (top). Signals representing Na(B3N2) are marked with grey stripes (top). For comparison PXD patterns of $NaLi(AB)_2$ and Na(B3N2) are shown (bottom).

10. Alkali metal M(B3N2) phases reported in the previous studies

In some previous papers authors have presented experimental results characterizing alkali metal (B3N2) phases (at that time, the chemical identity of these phases has not yet been established). We show comparison of previously reported PXD patterns of alkali metal M(B3N2) phases with data collected in present paper.

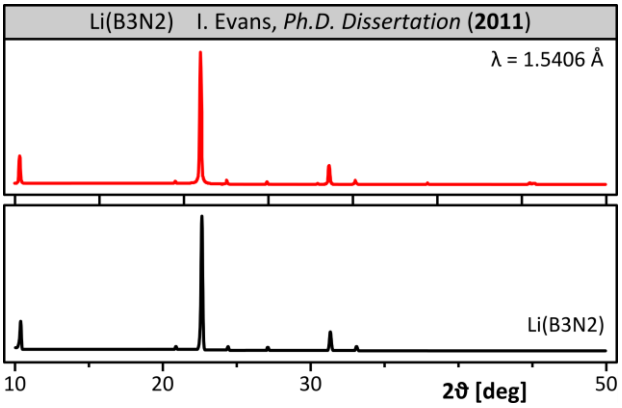

Fig. S10.1. PXD powder pattern of Li(B3N2) presented by I. Evans in his Ph.D. Dissertation in 2011 (top). For comparison a PXD pattern of Li(B3N2) obtained by us is shown below (bottom).

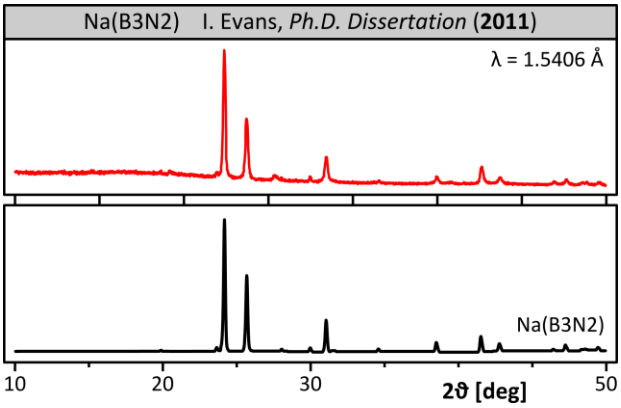

Fig. S10.2. PXD powder pattern of Na(B3N2) presented by I. Evans in his Ph.D. Dissertation in 2011 (top). For comparison a PXD pattern of Na(B3N2) obtained by us is shown below (bottom).

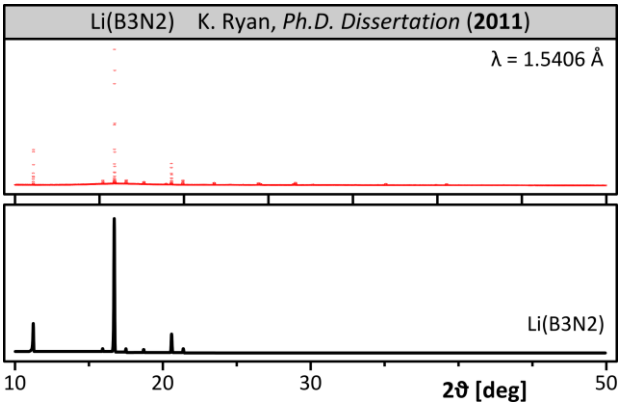

Fig. S10.3. PXD powder pattern of Li(B3N2) presented by K. Ryan in her Ph.D. Dissertation in 2011 (top). For comparison a PXD pattern of Li(B3N2) obtained by us is shown below (bottom).

11. Rietveld refinement of crystal structures of alkali metal M(B3N2) phases::

We have determined refined crystal structure of Li(B3N2) and Na(B3N2) form PXD pattern (λ ~ 1.789 Å) using JANA2006.

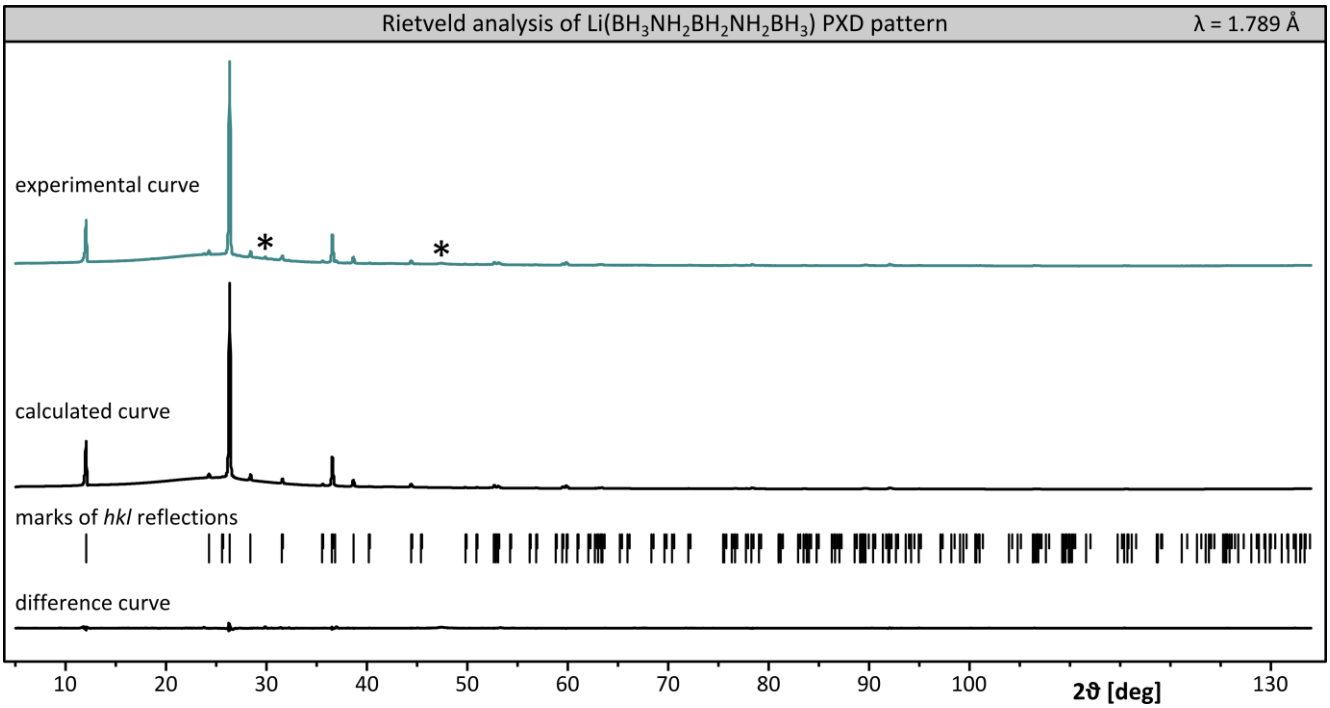

Fig. S11.1. Rietveld plot of Li($BH_3NH_2BH_2NH_2BH_3$) phase. The diffraction peaks from unidentified impurities have been marked with asterisk (*). CoKα, λ = 1.789Å.

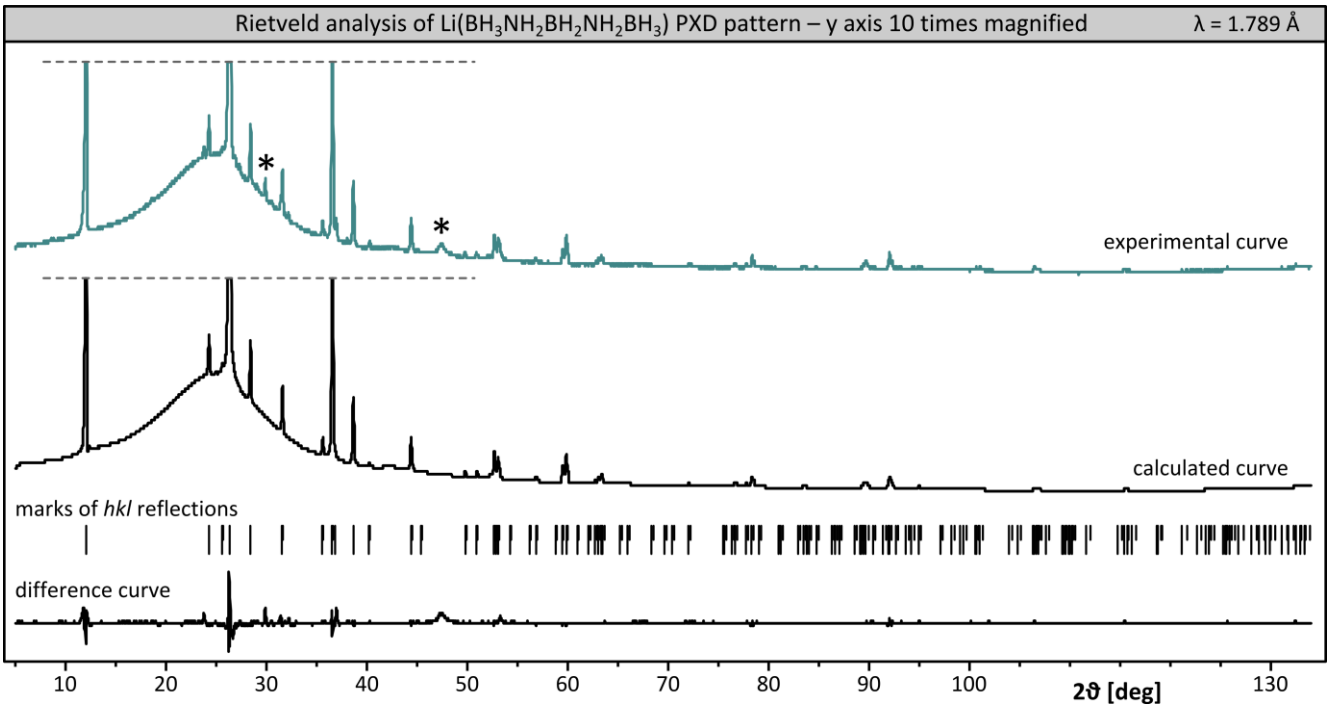

Fig. S11.2. Rietveld plot of Li($BH_3NH_2BH_2NH_2BH_3$) phase with magnified y axes. The diffraction peaks from unidentified impurities have been marked with asterisk (*). CoKα, λ = 1.789Å.

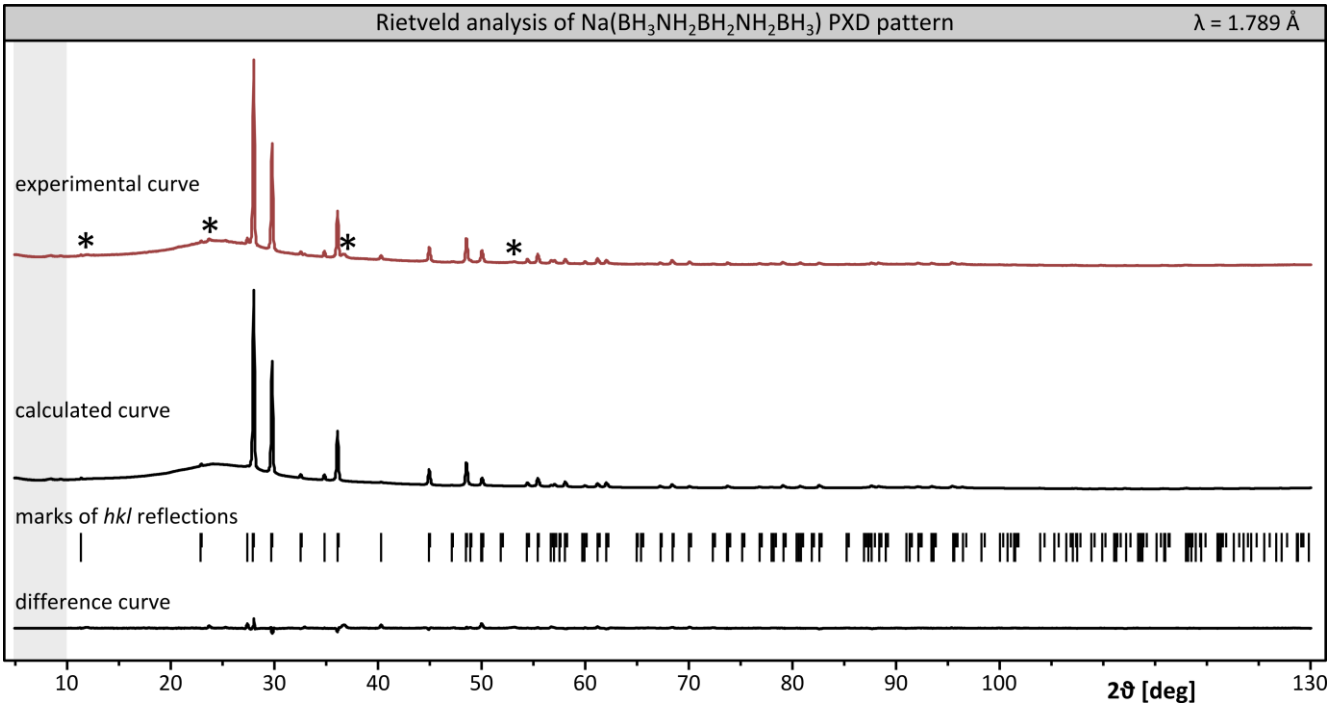

Fig. S11.3. Rietveld plot of $Na(BH_3NH_2BH_2NH_2BH_3)$ phase. The diffraction peaks from unidentified impurities have been marked with asterisk (*). CoKα, λ = 1.789Å.

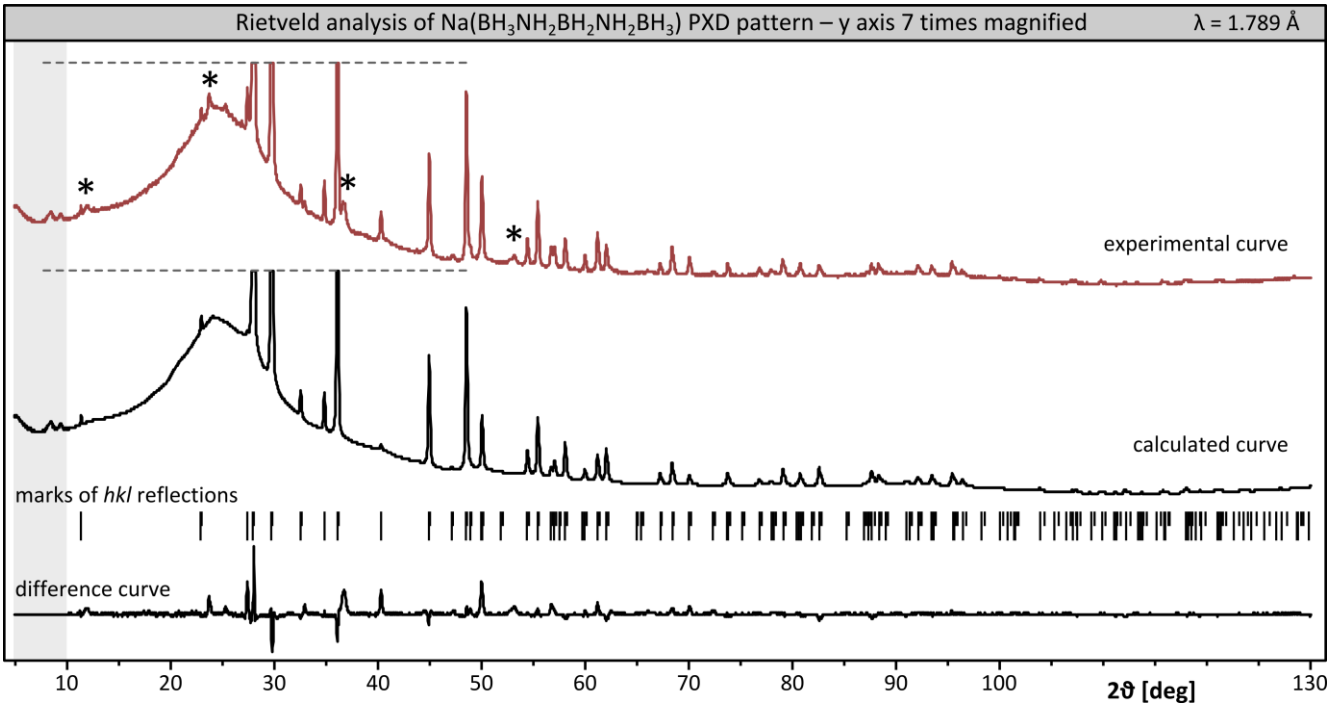

Fig. S11.4. Rietveld plot of $Na(BH_3NH_2BH_2NH_2BH_3)$ phase with magnified y axes. The diffraction peaks from unidentified impurities have been marked with asterisk (*). CoKα, λ = 1.789Å.

12. Quantitative phase analysis of the heated and aged amidoborane samples:

We detected formation of Na(B3N2) in the samples of sodium amidoborane aged at room temperature or heated to 55°C. In both cases *c.a.* 10% of the sample was transformed to Na(B3N2).

Table S12. Results of Rietveld analysis of samples of sodium amidoborane: (i) as synthesized, (ii) aged for 3 days at 25°C and (iii) stored at –35°C for three days and after that heated and measured at 55°C.

NaAB sample	NaAB [wt%]	Na(B3N2) [wt%]	wRp [%]	cRp	R(obs) NaAB	R(obs) Na(B3N2)
fresh	100	traces	6.02	16.81	2.83	1
aged 3 days (RT)	89.1(6)	10.9(5)	5.09	14.79	2.86	2.65
heated to 55°C	89.1(3)	10.9(2)	5.16	17.05	2.99	2.55

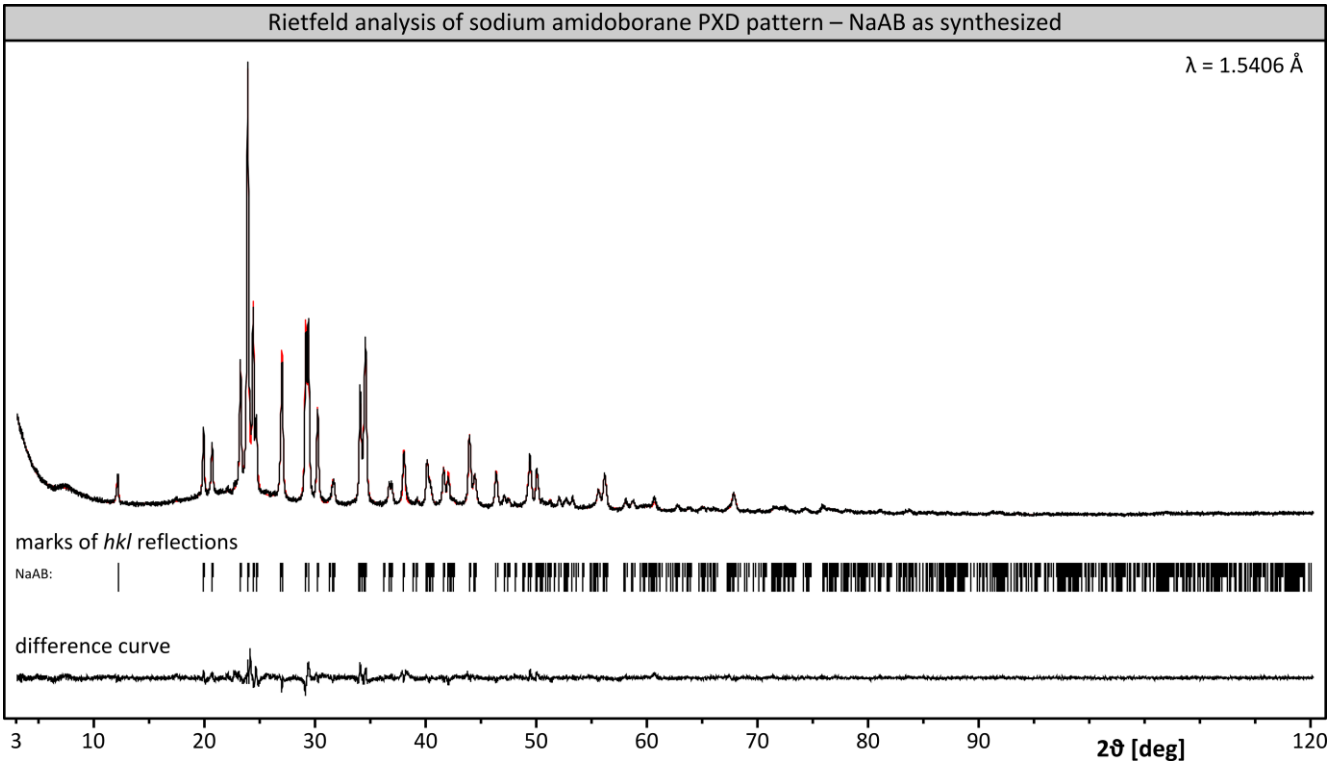

Fig S12.1. Rietfeld analysis of samples of as synthesized sodium amidoborane: experimental curve (black, top), calculated curve (red, top), marks of *hkl* reflections (middle), differential curve (bottom).

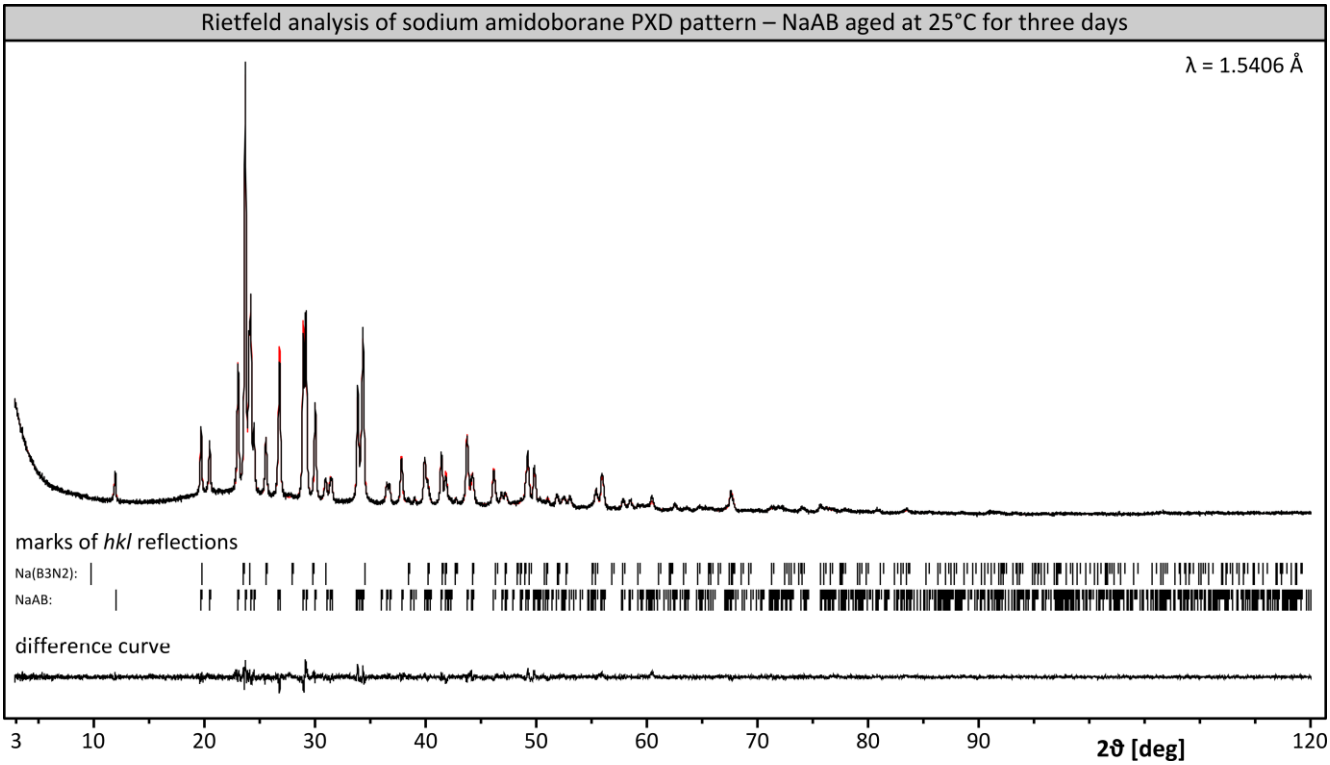

Fig S12.2. Rietfeld analysis of samples of sodium amidoborane aged for 3 days at 25°C: experimental curve (black, top), calculated curve (red, top), marks of *hkl* reflections (middle), differential curve (bottom).

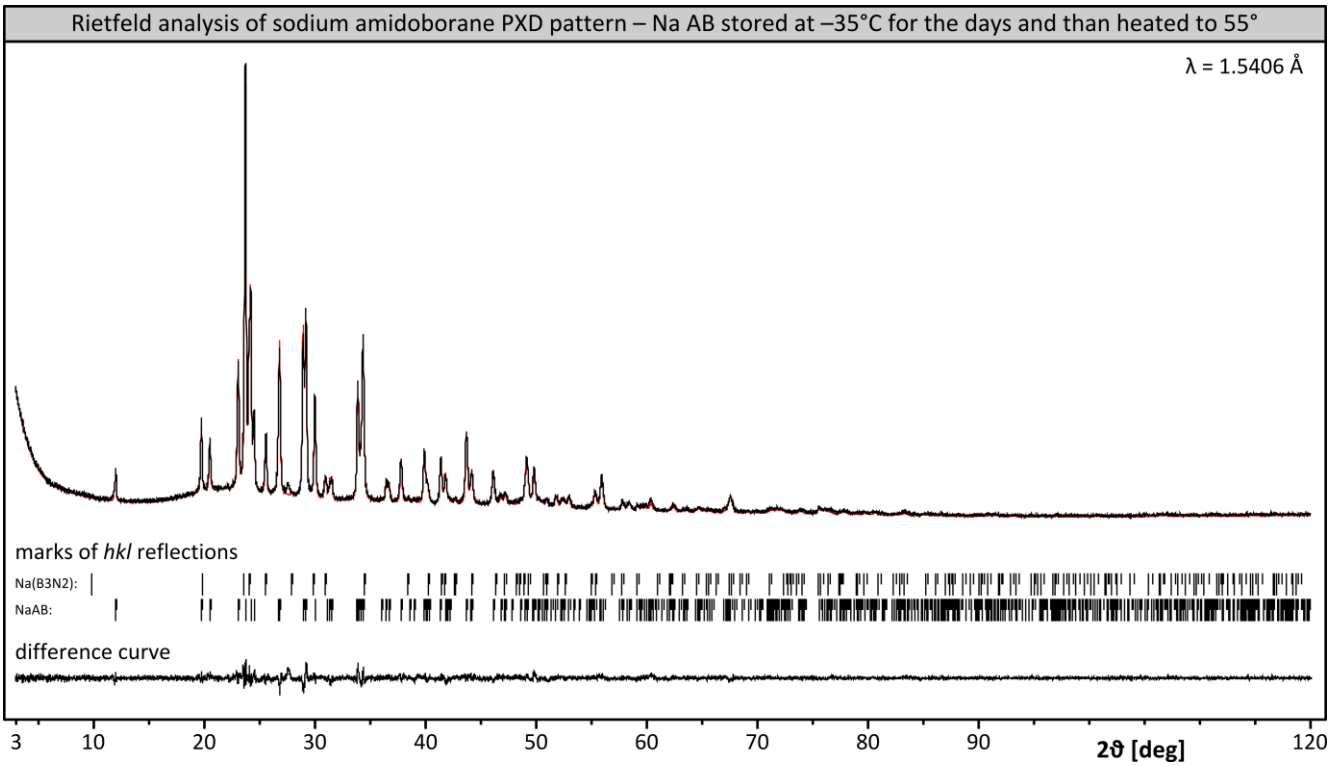

Fig S12.3. Rietfeld analysis of samples of sodium amidoborane stored at –35°C for three days and then heated and measured at 55°C: experimental curve (black, top), calculated curve (red, top), marks of *hkl* reflections (middle), differential curve (bottom).

13. Crystal structure of Na(B3N2) determined from single crystal x-ray diffraction:
The X-ray structures were measured in the Crystallography Unit of the Physical Chemistry Laboratory at the Faculty of Chemistry, the University of Warsaw.

The single crystal of Na(B3N2) was sealed in glass capillaries to protect them from moisture and than mounted on the goniometer of the diffractometer equipped with LT device. During measurements of all the crystals the temperature was set to 100 Kto protect the crystals from possible decomposition. All measurementswere performed on a KM4CCD k-axis diffractometer with graphite-monochromated MoKa radiation. The data were corrected for Lorentz and polarization effects. Empirical correction for absorption was applied [S1]. Data reduction and analysis were carried out with the Oxford Diffraction programs [S2]. The structure was solved by direct methods [S3] and refined using SHELXL [S4]. The refinement was based on F2. Scattering factors were taken from Tables 6.1.1.4 and 4.2.4.2 in [S5]. Hydrogen atoms were omited from the structure model.

The crystal structure exhibited severe disorder of the anionic (BNBNB) sublattice (Figure S13.1) and it will not be analyzed here in detail. However, it constituted a very valuable starting model for structure solution from powder data (as described in the main paper).

S1. CrysAlis RED, Agilent Technologies, Version 1.171.35.15. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
[S2] CrysAlis CCD, Agilent Technologies, Version 1.171.35.15; CrysAlis RED, Agilent Technologies, Version 1.171.35.15/1.171.35.11.
[S3] G.M. Sheldrick, Acta Crystallographica Section A: Foundations 46 (1990) 467–473.
[S4] G.M. Sheldrick, SHELXL93. Program for the Refinement of Crystal Structures, Univ. of Go¨ ttingen, Germany.
[S5] A.J.C. Wilson (Ed.), International Tables for Crystallography, vol. C, Kluwer, Dordrecht, 1992.

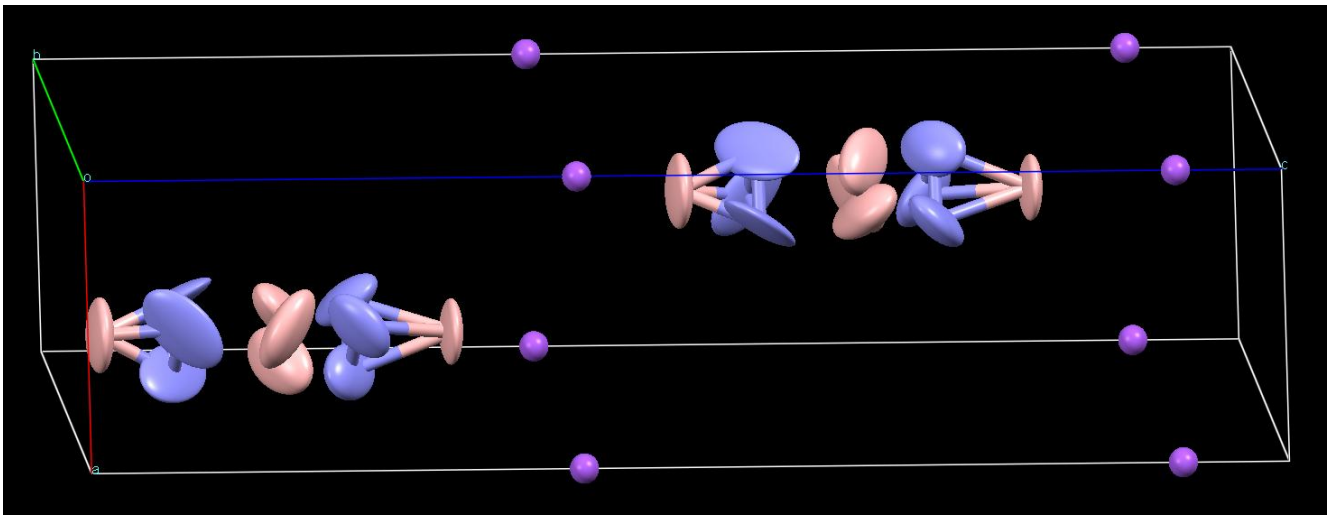

Fig S13.1. The provisional unit cell of Na(B3N2) phase as derived from the single crystal data at 100 K).

14. Results of the quantum-mechanical calculations for two isomeric forms of the "B3N2" anion:

Table S14.1. C_{2v} geometry optimization (MP2/6-311++G**) of $BH_3NH_2BH_2NH_2BH_3^-$ anion.

atom	X	Y	Z
H	–1.01168100	2.87678200	0.91874400
H	0.00000000	3.56622100	–0.68681200
H	1.01168100	2.87678200	0.91874400
H	–0.81103900	1.25093200	–1.02634000
H	0.81103900	1.25093200	–1.02634000
H	–1.01957700	0.00000000	1.18072700
H	1.01957700	0.00000000	1.18072700
H	0.81103900	–1.25093200	–1.02634000
H	–0.81103900	–1.25093200	–1.02634000
H	–1.01168100	–2.87678200	0.91874400
H	0.00000000	–3.56622100	–0.68681200
H	1.01168100	–2.87678200	0.91874400
N	0.00000000	1.28674800	–0.40924000
N	0.00000000	–1.28674800	–0.40924000
B	0.00000000	2.77277000	0.25094100
B	0.00000000	0.00000000	0.53250100
B	0.00000000	–2.77277000	0.25094100

Table S14.2. C_1 geometry optimization (MP2/6-311++G**) of $BH_3NH_2BH_2NH_2BH_3^-$ anion.

atom	X	Y	Z
N	0.96349700	–0.32870900	–0.14221000
H	0.79017300	–0.60073800	–1.10882300
H	0.62107700	–1.11779900	0.40482300
B	2.56748500	–0.21354500	0.04319100
H	2.79014000	0.07986000	1.20427900
B	0.07689800	0.91460100	0.21926800
H	0.10587000	1.09620700	1.41681600
H	0.43913900	1.88089800	–0.42554200
H	2.96400800	0.64504300	–0.72810900
N	–1.44649500	0.58309000	–0.17711700
H	–2.01756300	1.27170000	0.30895000
H	–1.59072100	0.78085900	–1.16613700
B	–2.06846400	–0.87610000	0.13265900
H	–1.54022700	–1.67133700	–0.62953100
H	–1.82588400	–1.14205300	1.29691500
H	–3.27401700	–0.81706300	–0.07595100
H	3.03939400	–1.31102600	–0.23799200

Vibrational frequencies (MP2/6-311++G**) for the C_{2v} isomer of $BH_3NH_2BH_2NH_2BH_3^-$.

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3						
	A2	B1	A1						
Frequencies --	52.2092	85.5593	150.9791						
Red. masses --	1.4054	2.3172	2.5305						
Frc consts --	0.0023	0.0100	0.0340						
IR Inten --	0.0000	10.4916	27.4568						
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 1	-0.25	0.00	-0.29	-0.25	-0.12	-0.10	0.00	-0.23	0.21
2 1	0.21	0.00	0.00	-0.18	0.00	0.00	0.00	0.12	0.36
3 1	-0.25	0.00	0.29	-0.25	0.12	0.10	0.00	-0.23	0.21
4 1	0.22	-0.02	-0.14	0.04	-0.11	0.02	0.00	0.13	-0.11
5 1	0.22	0.02	0.14	0.04	0.11	-0.02	0.00	0.13	-0.11
6 1	0.00	0.08	0.00	0.39	0.00	0.21	0.00	0.00	-0.18
7 1	0.00	-0.08	0.00	0.39	0.00	-0.21	0.00	0.00	-0.18
8 1	-0.22	0.02	-0.14	0.04	-0.11	-0.02	0.00	-0.13	-0.11
9 1	-0.22	-0.02	0.14	0.04	0.11	0.02	0.00	-0.13	-0.11
10 1	0.25	0.00	0.29	-0.25	0.12	-0.10	0.00	0.23	0.21
11 1	-0.21	0.00	0.00	-0.18	0.00	0.00	0.00	-0.12	0.36
12 1	0.25	0.00	-0.29	-0.25	-0.12	0.10	0.00	0.23	0.21
13 7	0.11	0.00	0.00	0.05	0.00	0.00	0.00	0.04	-0.11
14 7	-0.11	0.00	0.00	0.05	0.00	0.00	0.00	-0.04	-0.11
15 5	-0.06	0.00	0.00	-0.17	0.00	0.00	0.00	-0.09	0.19
16 5	0.00	0.00	0.00	0.25	0.00	0.00	0.00	0.00	-0.18
17 5	0.06	0.00	0.00	-0.17	0.00	0.00	0.00	0.09	0.19

	4	5	6						
	B1	A2	B2						
Frequencies --	172.8602	196.2486	291.9933						
Red. masses --	1.1217	1.2914	2.6698						
Frc consts --	0.0197	0.0293	0.1341						
IR Inten --	14.3400	0.0000	2.8094						
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 1	-0.13	0.17	-0.28	0.11	-0.20	0.25	0.00	0.28	-0.10
2 1	0.43	0.00	0.00	-0.41	0.00	0.00	0.00	-0.12	-0.27
3 1	-0.13	-0.17	0.28	0.11	0.20	-0.25	0.00	0.28	-0.10
4 1	-0.10	0.02	0.07	0.18	-0.02	-0.10	0.01	-0.04	0.18
5 1	-0.10	-0.02	-0.07	0.18	0.02	0.10	-0.01	-0.04	0.18
6 1	0.12	0.00	0.12	0.00	0.08	0.00	0.00	-0.30	0.00
7 1	0.12	0.00	-0.12	0.00	-0.08	0.00	0.00	-0.30	0.00
8 1	-0.10	0.02	-0.07	-0.18	0.02	-0.10	0.01	-0.04	-0.18
9 1	-0.10	-0.02	0.07	-0.18	-0.02	0.10	-0.01	-0.04	-0.18
10 1	-0.13	-0.17	-0.28	-0.11	-0.20	-0.25	0.00	0.28	0.10

11	1	0.43	0.00	0.00	0.41	0.00	0.00	0.00	-0.12	0.27
12	1	-0.13	0.17	0.28	-0.11	0.20	0.25	0.00	0.28	0.10
13	7	-0.05	0.00	0.00	0.10	0.00	0.00	0.00	-0.03	0.20
14	7	-0.05	0.00	0.00	-0.10	0.00	0.00	0.00	-0.03	-0.20
15	5	0.04	0.00	0.00	-0.03	0.00	0.00	0.00	0.11	-0.07
16	5	0.04	0.00	0.00	0.00	0.00	0.00	0.00	-0.17	0.00
17	5	0.04	0.00	0.00	0.03	0.00	0.00	0.00	0.11	0.07

	7	8	9
	A1	B1	A2
Frequencies --	326.7107	604.9257	611.9930
Red. masses --	3.5448	1.0628	1.1215
Frc consts --	0.2229	0.2291	0.2475
IR Inten --	0.0004	0.0532	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.00	0.30	0.03	-0.07	-0.13	-0.08	0.08	0.19	0.10
2	1	0.00	0.21	-0.01	-0.05	0.00	0.00	0.09	0.00	0.00
3	1	0.00	0.30	0.03	-0.07	0.13	0.08	0.08	-0.19	-0.10
4	1	0.00	0.27	0.00	-0.21	0.03	0.33	0.21	-0.07	-0.35
5	1	0.00	0.27	0.00	-0.21	-0.03	-0.33	0.21	0.07	0.35
6	1	0.00	0.00	-0.11	-0.19	0.00	-0.31	0.00	-0.19	0.00
7	1	0.00	0.00	-0.11	-0.19	0.00	0.31	0.00	0.19	0.00
8	1	0.00	-0.27	0.00	-0.21	0.03	-0.33	-0.21	0.07	-0.35
9	1	0.00	-0.27	0.00	-0.21	-0.03	0.33	-0.21	-0.07	0.35
10	1	0.00	-0.30	0.03	-0.07	0.13	-0.08	-0.08	0.19	-0.10
11	1	0.00	-0.21	-0.01	-0.05	0.00	0.00	-0.09	0.00	0.00
12	1	0.00	-0.30	0.03	-0.07	-0.13	0.08	-0.08	-0.19	0.10
13	7	0.00	0.18	0.02	0.04	0.00	0.00	-0.07	0.00	0.00
14	7	0.00	-0.18	0.02	0.04	0.00	0.00	0.07	0.00	0.00
15	5	0.00	0.27	0.04	0.01	0.00	0.00	-0.01	0.00	0.00
16	5	0.00	0.00	-0.11	0.02	0.00	0.00	0.00	0.00	0.00
17	5	0.00	-0.27	0.04	0.01	0.00	0.00	0.01	0.00	0.00

	10	11	12
	B2	A1	B1
Frequencies --	720.6843	751.4170	780.3393
Red. masses --	3.9657	2.0675	1.1641
Frc consts --	1.2136	0.6878	0.4177
IR Inten --	0.5158	0.2337	0.0214

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.00	-0.07	-0.10	-0.02	0.15	-0.06	0.07	0.27	0.12
2	1	0.00	-0.38	-0.21	0.00	-0.42	-0.27	0.12	0.00	0.00
3	1	0.00	-0.07	-0.10	0.02	0.15	-0.06	0.07	-0.27	-0.12
4	1	0.00	0.08	0.17	0.00	0.21	0.10	0.01	-0.27	-0.02
5	1	0.00	0.08	0.17	0.00	0.21	0.10	0.01	0.27	0.02
6	1	0.00	0.26	0.00	0.00	0.00	-0.21	-0.14	0.00	-0.35
7	1	0.00	0.26	0.00	0.00	0.00	-0.21	-0.14	0.00	0.35
8	1	0.00	0.08	-0.17	0.00	-0.21	0.10	0.01	-0.27	0.02

9	1	0.00	0.08	-0.17	0.00	-0.21	0.10	0.01	0.27	-0.02
10	1	0.00	-0.07	0.10	-0.02	-0.15	-0.06	0.07	-0.27	0.12
11	1	0.00	-0.38	0.21	0.00	0.42	-0.27	0.12	0.00	0.00
12	1	0.00	-0.07	0.10	0.02	-0.15	-0.06	0.07	0.27	-0.12
13	7	0.00	0.09	0.17	0.00	0.00	0.11	-0.02	0.00	0.00
14	7	0.00	0.09	-0.17	0.00	0.00	0.11	-0.02	0.00	0.00
15	5	0.00	-0.24	-0.07	0.00	-0.10	0.01	-0.04	0.00	0.00
16	5	0.00	0.28	0.00	0.00	0.00	-0.23	0.10	0.00	0.00
17	5	0.00	-0.24	0.07	0.00	0.10	0.01	-0.04	0.00	0.00

	13	14	15
	B2	A1	A2
Frequencies --	840.5961	850.0462	856.3513
Red. masses --	3.1404	4.4380	1.0828
Frc consts --	1.3074	1.8894	0.4678
IR Inten --	143.9528	2.9861	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.02	-0.25	-0.04	0.01	-0.26	-0.09	0.06	0.25	0.12
2	1	0.00	0.26	0.17	0.00	0.08	0.07	0.10	0.00	0.00
3	1	-0.02	-0.25	-0.04	-0.01	-0.26	-0.09	0.06	-0.25	-0.12
4	1	0.01	0.14	-0.03	0.00	0.29	0.03	-0.04	-0.27	0.10
5	1	-0.01	0.14	-0.03	0.00	0.29	0.03	-0.04	0.27	-0.10
6	1	0.00	-0.38	0.00	0.00	0.00	0.15	0.00	0.39	0.00
7	1	0.00	-0.38	0.00	0.00	0.00	0.15	0.00	-0.39	0.00
8	1	0.01	0.14	0.03	0.00	-0.29	0.03	0.04	0.27	0.10
9	1	-0.01	0.14	0.03	0.00	-0.29	0.03	0.04	-0.27	-0.10
10	1	-0.02	-0.25	0.04	0.01	0.26	-0.09	-0.06	0.25	-0.12
11	1	0.00	0.26	-0.17	0.00	-0.08	0.07	-0.10	0.00	0.00
12	1	0.02	-0.25	0.04	-0.01	0.26	-0.09	-0.06	-0.25	0.12
13	7	0.00	0.20	-0.01	0.00	0.28	0.03	0.03	0.00	0.00
14	7	0.00	0.20	0.01	0.00	-0.28	0.03	-0.03	0.00	0.00
15	5	0.00	-0.10	-0.12	0.00	-0.18	-0.14	-0.05	0.00	0.00
16	5	0.00	-0.25	0.00	0.00	0.00	0.18	0.00	0.00	0.00
17	5	0.00	-0.10	0.12	0.00	0.18	-0.14	0.05	0.00	0.00

	16	17	18
	B2	A1	B1
Frequencies --	900.6181	992.5515	1077.7618
Red. masses --	1.2790	1.7139	1.6444
Frc consts --	0.6112	0.9948	1.1254
IR Inten --	0.3065	24.9159	68.0993

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.02	0.22	-0.03	0.03	-0.30	0.01	-0.05	-0.31	-0.16
2	1	0.00	-0.33	-0.21	0.00	0.35	0.21	-0.10	0.00	0.00
3	1	0.02	0.22	-0.03	-0.03	-0.30	0.01	-0.05	0.31	0.16
4	1	0.00	0.33	-0.07	0.00	-0.17	0.11	0.07	-0.08	-0.23
5	1	0.00	0.33	-0.07	0.00	-0.17	0.11	0.07	0.08	0.23
6	1	0.00	0.05	0.00	-0.03	0.00	-0.20	-0.07	0.00	-0.30

7	1	0.00	0.05	0.00	0.03	0.00	-0.20	-0.07	0.00	0.30
8	1	0.00	0.33	0.07	0.00	0.17	0.11	0.07	-0.08	0.23
9	1	0.00	0.33	0.07	0.00	0.17	0.11	0.07	0.08	-0.23
10	1	0.02	0.22	0.03	0.03	0.30	0.01	-0.05	0.31	-0.16
11	1	0.00	-0.33	0.21	0.00	-0.35	0.21	-0.10	0.00	0.00
12	1	-0.02	0.22	0.03	-0.03	0.30	0.01	-0.05	-0.31	0.16
13	7	0.00	0.01	-0.05	0.00	0.00	0.11	-0.11	0.00	0.00
14	7	0.00	0.01	0.05	0.00	0.00	0.11	-0.11	0.00	0.00
15	5	0.00	-0.04	0.05	0.00	0.04	-0.09	0.09	0.00	0.00
16	5	0.00	-0.10	0.00	0.00	0.00	-0.15	0.13	0.00	0.00
17	5	0.00	-0.04	-0.05	0.00	-0.04	-0.09	0.09	0.00	0.00

	19	20	21
	A2	B2	A2
Frequencies --	1092.4998	1126.5992	1169.3327
Red. masses --	1.2811	1.2789	1.0429
Frc consts --	0.9009	0.9564	0.8402
IR Inten --	0.0000	1.7641	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.04	-0.20	-0.11	0.02	-0.15	0.01	-0.01	-0.19	-0.05
2	1	-0.08	0.00	0.00	0.00	0.19	0.09	0.04	0.00	0.00
3	1	-0.04	0.20	0.11	-0.02	-0.15	0.01	-0.01	0.19	0.05
4	1	0.05	-0.05	-0.17	0.00	0.25	0.03	-0.01	-0.41	0.03
5	1	0.05	0.05	0.17	0.00	0.25	0.03	-0.01	0.41	-0.03
6	1	0.00	0.55	0.00	0.00	0.52	0.00	0.00	-0.27	0.00
7	1	0.00	-0.55	0.00	0.00	0.52	0.00	0.00	0.27	0.00
8	1	-0.05	0.05	-0.17	0.00	0.25	-0.03	0.01	0.41	0.03
9	1	-0.05	-0.05	0.17	0.00	0.25	-0.03	0.01	-0.41	-0.03
10	1	0.04	-0.20	0.11	-0.02	-0.15	-0.01	0.01	-0.19	0.05
11	1	0.08	0.00	0.00	0.00	0.19	-0.09	-0.04	0.00	0.00
12	1	0.04	0.20	-0.11	0.02	-0.15	-0.01	0.01	0.19	-0.05
13	7	-0.09	0.00	0.00	0.00	-0.05	0.05	0.00	0.00	0.00
14	7	0.09	0.00	0.00	0.00	-0.05	-0.05	0.00	0.00	0.00
15	5	0.06	0.00	0.00	0.00	0.03	-0.05	0.04	0.00	0.00
16	5	0.00	0.00	0.00	0.00	-0.08	0.00	0.00	0.00	0.00
17	5	-0.06	0.00	0.00	0.00	0.03	0.05	-0.04	0.00	0.00

	22	23	24
	B2	A1	A1
Frequencies --	1175.3528	1199.2872	1215.5509
Red. masses --	1.2101	1.1661	1.1714
Frc consts --	0.9850	0.9882	1.0198
IR Inten --	770.2583	2.9476	59.1592

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.07	0.30	0.06	-0.06	-0.25	-0.05	0.28	0.13	0.34
2	1	0.00	0.12	0.14	0.00	-0.04	-0.08	0.00	0.12	0.06
3	1	-0.07	0.30	0.06	0.06	-0.25	-0.05	-0.28	0.13	0.34
4	1	0.01	-0.25	-0.01	0.00	0.29	-0.01	0.00	0.17	-0.01

5	1	-0.01	-0.25	-0.01	0.00	0.29	-0.01	0.00	0.17	-0.01
6	1	0.00	0.37	0.00	0.23	0.00	0.35	0.02	0.00	0.02
7	1	0.00	0.37	0.00	-0.23	0.00	0.35	-0.02	0.00	0.02
8	1	0.01	-0.25	0.01	0.00	-0.29	-0.01	0.00	-0.17	-0.01
9	1	-0.01	-0.25	0.01	0.00	-0.29	-0.01	0.00	-0.17	-0.01
10	1	-0.07	0.30	-0.06	-0.06	0.25	-0.05	0.28	-0.13	0.34
11	1	0.00	0.12	-0.14	0.00	0.04	-0.08	0.00	-0.12	0.06
12	1	0.07	0.30	-0.06	0.06	0.25	-0.05	-0.28	-0.13	0.34
13	7	0.00	0.04	0.00	0.00	-0.06	0.01	0.00	-0.04	0.00
14	7	0.00	0.04	0.00	0.00	0.06	0.01	0.00	0.04	0.00
15	5	0.00	-0.06	0.00	0.00	0.06	-0.01	0.00	-0.02	-0.07
16	5	0.00	-0.09	0.00	0.00	0.00	-0.03	0.00	0.00	0.01
17	5	0.00	-0.06	0.00	0.00	-0.06	-0.01	0.00	0.02	-0.07

	25	26	27
	B2	B1	A2
Frequencies --	1218.6200	1221.3102	1225.4622
Red. masses --	1.0880	1.0466	1.0801
Frc consts --	0.9520	0.9198	0.9557
IR Inten --	6.6142	20.3400	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.29	-0.02	-0.39	0.05	-0.28	0.15	-0.06	0.24	-0.19
2	1	0.00	0.07	0.09	0.48	0.00	0.00	-0.53	0.00	0.00
3	1	0.29	-0.02	-0.39	0.05	0.28	-0.15	-0.06	-0.24	0.19
4	1	0.00	-0.06	0.01	-0.01	-0.16	0.03	0.00	-0.06	0.01
5	1	0.00	-0.06	0.01	-0.01	0.16	-0.03	0.00	0.06	-0.01
6	1	0.00	0.09	0.00	0.01	0.00	0.08	0.00	-0.05	0.00
7	1	0.00	0.09	0.00	0.01	0.00	-0.08	0.00	0.05	0.00
8	1	0.00	-0.06	-0.01	-0.01	-0.16	-0.03	0.00	0.06	0.01
9	1	0.00	-0.06	-0.01	-0.01	0.16	0.03	0.00	-0.06	-0.01
10	1	0.29	-0.02	0.39	0.05	0.28	0.15	0.06	0.24	0.19
11	1	0.00	0.07	-0.09	0.48	0.00	0.00	0.53	0.00	0.00
12	1	-0.29	-0.02	0.39	0.05	-0.28	-0.15	0.06	-0.24	-0.19
13	7	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00
14	7	0.00	0.01	0.00	0.00	0.00	0.00	-0.01	0.00	0.00
15	5	0.00	0.00	0.06	-0.03	0.00	0.00	0.06	0.00	0.00
16	5	0.00	-0.02	0.00	-0.04	0.00	0.00	0.00	0.00	0.00
17	5	0.00	0.00	-0.06	-0.03	0.00	0.00	-0.06	0.00	0.00

	28	29	30
	A1	B2	B1
Frequencies --	1225.7178	1235.2562	1241.9509
Red. masses --	1.1204	1.2578	1.1784
Frc consts --	0.9918	1.1307	1.0709
IR Inten --	6.1570	0.6262	6.8166

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.11	0.22	-0.22	0.01	0.24	-0.06	0.03	0.00	0.13
2	1	0.00	0.36	0.32	0.00	0.35	0.31	0.23	0.00	0.00

3	1	0.11	0.22	-0.22	-0.01	0.24	-0.06	0.03	0.00	-0.13
4	1	-0.01	0.15	0.01	-0.02	0.20	0.02	0.02	0.42	-0.07
5	1	0.01	0.15	0.01	0.02	0.20	0.02	0.02	-0.42	0.07
6	1	0.04	0.00	0.05	0.00	-0.25	0.00	-0.03	0.00	-0.20
7	1	-0.04	0.00	0.05	0.00	-0.25	0.00	-0.03	0.00	0.20
8	1	0.01	-0.15	0.01	-0.02	0.20	-0.02	0.02	0.42	0.07
9	1	-0.01	-0.15	0.01	0.02	0.20	-0.02	0.02	-0.42	-0.07
10	1	-0.11	-0.22	-0.22	-0.01	0.24	0.06	0.03	0.00	0.13
11	1	0.00	-0.36	0.32	0.00	0.35	-0.31	0.23	0.00	0.00
12	1	0.11	-0.22	-0.22	0.01	0.24	0.06	0.03	0.00	-0.13
13	7	0.00	-0.04	0.01	0.00	-0.06	0.00	-0.02	0.00	0.00
14	7	0.00	0.04	0.01	0.00	-0.06	0.00	-0.02	0.00	0.00
15	5	0.00	-0.05	0.00	0.00	-0.06	-0.03	-0.06	0.00	0.00
16	5	0.00	0.00	-0.01	0.00	0.09	0.00	0.10	0.00	0.00
17	5	0.00	0.05	0.00	0.00	-0.06	0.03	-0.06	0.00	0.00

	31	32	33
	A1	B2	A1
Frequencies --	1242.8001	1598.0324	1611.8588
Red. masses --	1.2046	1.0884	1.0845
Frc consts --	1.0962	1.6376	1.6601
IR Inten --	28.3615	0.0058	47.4961

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.04	0.12	0.04	0.00	0.00	-0.01	0.00	0.00	0.01
2	1	0.00	0.01	0.04	0.00	0.01	0.01	0.00	-0.01	-0.01
3	1	-0.04	0.12	0.04	0.00	0.00	-0.01	0.00	0.00	0.01
4	1	0.01	-0.23	0.00	0.31	0.00	-0.39	-0.31	0.01	0.39
5	1	-0.01	-0.23	0.00	-0.31	0.00	-0.39	0.31	0.01	0.39
6	1	0.36	0.00	0.46	0.00	-0.02	0.00	0.01	0.00	0.02
7	1	-0.36	0.00	0.46	0.00	-0.02	0.00	-0.01	0.00	0.02
8	1	-0.01	0.23	0.00	0.31	0.00	0.39	0.31	-0.01	0.39
9	1	0.01	0.23	0.00	-0.31	0.00	0.39	-0.31	-0.01	0.39
10	1	0.04	-0.12	0.04	0.00	0.00	0.01	0.00	0.00	0.01
11	1	0.00	-0.01	0.04	0.00	0.01	-0.01	0.00	0.01	-0.01
12	1	-0.04	-0.12	0.04	0.00	0.00	0.01	0.00	0.00	0.01
13	7	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.00	-0.05
14	7	0.00	-0.05	0.00	0.00	0.00	-0.05	0.00	0.00	-0.05
15	5	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	5	0.00	0.00	-0.11	0.00	0.01	0.00	0.00	0.00	-0.01
17	5	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00

	34	35	36
	B2	A1	B2
Frequencies --	2366.7959	2370.6895	2445.9493
Red. masses --	1.0650	1.0664	1.0659
Frc consts --	3.5151	3.5312	3.7570
IR Inten --	478.2722	269.3894	13.8884

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z

1	1	-0.07	0.00	0.06	0.06	0.00	-0.06	-0.41	0.04	0.26
2	1	0.00	0.45	-0.53	0.00	-0.45	0.53	0.00	-0.07	0.07
3	1	0.07	0.00	0.06	-0.06	0.00	-0.06	0.41	0.04	0.26
4	1	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
5	1	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
6	1	0.00	0.00	0.00	-0.02	0.00	0.01	0.00	0.00	0.00
7	1	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00
8	1	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
9	1	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00	0.00
10	1	0.07	0.00	-0.06	0.06	0.00	-0.06	0.41	0.04	-0.26
11	1	0.00	0.45	0.53	0.00	0.45	0.53	0.00	-0.07	-0.07
12	1	-0.07	0.00	-0.06	-0.06	0.00	-0.06	-0.41	0.04	-0.26
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	5	0.00	-0.04	0.04	0.00	0.04	-0.04	0.00	0.00	-0.05
16	5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	5	0.00	-0.04	-0.04	0.00	-0.04	-0.04	0.00	0.00	0.05

	37	38	39
	A1	A2	B1
Frequencies --	2446.1793	2475.5075	2475.8511
Red. masses --	1.0640	1.1131	1.1133
Frc consts --	3.7513	4.0188	4.0207
IR Inten --	304.7919	0.0000	530.0815

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.41	-0.04	-0.26	-0.41	0.04	0.28	0.40	-0.04	-0.28
2	1	0.00	0.06	-0.07	0.02	0.00	0.00	-0.02	0.00	0.00
3	1	-0.41	-0.04	-0.26	-0.41	-0.04	-0.28	0.40	0.04	0.28
4	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	1	-0.12	0.00	0.07	0.00	0.00	0.00	-0.08	0.00	0.05
7	1	0.12	0.00	0.07	0.00	0.00	0.00	-0.08	0.00	-0.05
8	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	1	0.41	0.04	-0.26	0.41	0.04	-0.28	0.40	0.04	-0.28
11	1	0.00	-0.06	-0.07	-0.02	0.00	0.00	-0.02	0.00	0.00
12	1	-0.41	0.04	-0.26	0.41	-0.04	0.28	0.40	-0.04	0.28
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	5	0.00	0.00	0.05	0.07	0.00	0.00	-0.07	0.00	0.00
16	5	0.00	0.00	-0.01	0.00	0.00	0.00	0.01	0.00	0.00
17	5	0.00	0.00	0.05	-0.07	0.00	0.00	-0.07	0.00	0.00

	40	41	42
	A1	B1	A1
Frequencies --	2505.8726	2555.2550	3483.9622
Red. masses --	1.0528	1.1211	1.0504
Frc consts --	3.8950	4.3129	7.5118

IR Inten	--	185.9504			320.5491			1.2971		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.08	-0.01	-0.05	0.06	0.00	-0.04	0.00	0.00	0.00
2	1	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	1	-0.08	-0.01	-0.05	0.06	0.00	0.04	0.00	0.00	0.00
4	1	0.00	0.00	0.01	-0.01	-0.01	0.00	-0.41	-0.01	-0.28
5	1	0.00	0.00	0.01	-0.01	0.01	0.00	0.41	-0.01	-0.28
6	1	0.58	0.00	-0.37	0.58	0.00	-0.38	0.00	0.00	0.00
7	1	-0.58	0.00	-0.37	0.58	0.00	0.38	0.00	0.00	0.00
8	1	0.00	0.00	0.01	-0.01	-0.01	0.00	0.41	0.01	-0.28
9	1	0.00	0.00	0.01	-0.01	0.01	0.00	-0.41	0.01	-0.28
10	1	0.08	0.01	-0.05	0.06	0.00	-0.04	0.00	0.00	0.00
11	1	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	1	-0.08	0.01	-0.05	0.06	0.00	0.04	0.00	0.00	0.00
13	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04
14	7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04
15	5	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00
16	5	0.00	0.00	0.07	-0.11	0.00	0.00	0.00	0.00	0.00
17	5	0.00	0.00	0.01	-0.01	0.00	0.00	0.00	0.00	0.00

	43	44	45
	B2	B1	A2
Frequencies --	3484.2397	3567.8663	3568.8975
Red. masses --	1.0518	1.0897	1.0906
Frc consts --	7.5234	8.1731	8.1845
IR Inten --	1.0951	4.8269	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	1	0.41	0.02	0.29	0.40	0.02	0.30	0.40	0.02	0.30
5	1	-0.41	0.02	0.29	0.40	-0.02	-0.30	0.40	-0.02	-0.30
6	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
7	1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
8	1	0.41	0.02	-0.29	0.40	0.02	-0.30	-0.40	-0.02	0.30
9	1	-0.41	0.02	-0.29	0.40	-0.02	0.30	-0.40	0.02	-0.30
10	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	7	0.00	0.00	-0.04	-0.06	0.00	0.00	-0.06	0.00	0.00
14	7	0.00	0.00	0.04	-0.06	0.00	0.00	0.06	0.00	0.00
15	5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00