

## **Additives in Protic-Hydridic Hydrogen Storage Compounds: A Molecular Study**

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Frisch, M. J.; et al. Gaussian 09 , Revision B.1; Gaussian: Wallingford, CT, USA, 2009.

Table (S6) : Atomic Hydrogen liberation Energy of all the steps (Units in eV/Mol)

Compound	1 <sup>st</sup> step	2 <sup>nd</sup> step	3 <sup>rd</sup> step	4 <sup>th</sup> step	5 <sup>th</sup> step	6 <sup>th</sup> step	7 <sup>th</sup> step	8 <sup>th</sup> step	9 <sup>th</sup> step	10 <sup>th</sup> step
NH <sub>3</sub> (-H <sub>N</sub> =4.92) NH <sub>2</sub>	NH <sub>2</sub> (-H <sub>N</sub> =6.46) NH	NH (-H <sub>N</sub> =4.34) N								
BH <sub>3</sub> (-H <sub>B</sub> =4.80) BH <sub>2</sub>	BH <sub>2</sub> (-H <sub>B</sub> =3.94) BH	BH (-H <sub>N</sub> =3.61) B								
LiNH <sub>2</sub> (-H <sub>N</sub> =4.92) LiNH	LiNH (-H <sub>N</sub> =6.45) LiN									
LiBH <sub>2</sub> (-H <sub>B</sub> =4.21) LiBH	LiBH (-H <sub>N</sub> =4.76) LiB									
NH <sub>3</sub> BH <sub>3</sub> (-H <sub>N</sub> =4.92) 1) NH <sub>2</sub> BH <sub>3</sub> (-H <sub>B</sub> =4.68) 2) NH <sub>3</sub> BH <sub>2</sub>	NH <sub>3</sub> BH <sub>2</sub> (-H <sub>N</sub> =2.03) 1) NH <sub>2</sub> BH <sub>2</sub> (-H <sub>B</sub> =4.68) 2) NH <sub>3</sub> BH	NH <sub>2</sub> BH <sub>2</sub> (-H <sub>B</sub> =4.81) 1) (-H <sub>N</sub> =5.47) 2) NHBH <sub>2</sub>	NH <sub>2</sub> BH (-H <sub>N</sub> =2.99) 1) NHBH (-H <sub>B</sub> =3.40) 2) NH <sub>2</sub> B	NHBH (-H <sub>B</sub> =5.10) 1) BNH (-H <sub>N</sub> =5.96) 2) NBH	BNH (-H <sub>N</sub> =6.42) 1) BN					
LiNH <sub>2</sub> BH <sub>3</sub> (-H <sub>B</sub> =4.50) 1) LiNH <sub>2</sub> BH <sub>2</sub>	LiNH <sub>2</sub> BH <sub>2</sub> (-H <sub>N</sub> =2.65) 1) LiNHBH <sub>2</sub>	LiNHBH <sub>2</sub> (-H <sub>B</sub> =4.52) 1) LiNHBH	LiNHBH (-H <sub>N</sub> =2.64) 1) LiNBH	LiNBH (-H <sub>N</sub> =4.98) LiNB						

(-H <sub>N</sub> =4.89) 2) LiNHBH <sub>3</sub>	(-H <sub>N</sub> =4.59) 2) LiNH <sub>2</sub> BH	(-H <sub>N</sub> =4.89) 2)LiNBH <sub>2</sub>	(-H <sub>B</sub> =3.30) 2)LiBNH						
LiBH <sub>2</sub> NH <sub>3</sub> (-H <sub>N</sub> =2.58) 1) LiBH <sub>2</sub> NH <sub>2</sub>  (-H <sub>B</sub> =4.30) 2) LiBHNH <sub>3</sub>									
LiNH <sub>2</sub> NH <sub>3</sub> (-H <sub>N2</sub> =4.66) 1) LiNH <sub>2</sub> NH <sub>2</sub>  (-H <sub>N1</sub> =4.88) 2) LiNHNH <sub>3</sub>	LiNH <sub>2</sub> NH <sub>2</sub> (-H <sub>N1</sub> =6.23) 1) LiNHNH <sub>2</sub>	LiNHNH <sub>2</sub> (-H <sub>N2</sub> =3.66) 1) LiNHNH	LiNHNH (-H <sub>N1</sub> =3.39) 1)LiNHNH	LiNNH (-H <sub>N2</sub> = 2.22) 1)LiNN					
LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub> (-H <sub>B</sub> =4.49) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> (-H <sub>N1</sub> =5.50) LiNHBH <sub>3</sub> .NH <sub>3</sub> (-H <sub>N2</sub> =6.14)	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> (-H <sub>N1</sub> =2.63) 1) LiNHBH <sub>2</sub> .NH <sub>3</sub>  (-H <sub>B</sub> =4.47) 2) LiNH <sub>2</sub> BHNH <sub>3</sub>	LiNHBH <sub>2</sub> .NH <sub>3</sub> (-H <sub>B</sub> =4.52) 1) LiNHBH.NH <sub>3</sub>  (-H <sub>N1</sub> =5.19) 2)LiNHBH <sub>2</sub> .NH <sub>2</sub>	LiNHBH.NH <sub>3</sub> (-H <sub>N2</sub> =2.57) 1) LiNBH.NH <sub>3</sub>  (-H <sub>B</sub> =2.92) 2) LiBNH.NH <sub>3</sub>	LiNBH.NH <sub>3</sub> (-H <sub>B</sub> =4.97) 1) LiNB.NH <sub>3</sub>  (-H <sub>N2</sub> =5.15) 2)LiNBH.NH <sub>2</sub>	LiNB.NH <sub>3</sub> (-H <sub>N2</sub> =6.51) LiNB.NH <sub>2</sub>	LiNB.NH <sub>2</sub> (-H <sub>N2</sub> =3.81) LiNB.NH	LiNB.NH (-H <sub>N2</sub> =4.24)		

LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>2</sub>	(-H <sub>N2</sub> =3.18) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>2</sub>	(-H <sub>N2</sub> =4.80) 3) LiNBH.NH <sub>3</sub>	(-H <sub>N1</sub> =4.48) 3)LiNHBH.NH <sub>2</sub>							
LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub> (-H <sub>B</sub> =4.49) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> (-H <sub>N1</sub> =5.50) LiNHBH <sub>3</sub> .NH <sub>3</sub> (-H <sub>N2</sub> =6.14) LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>2</sub>	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> (-H <sub>N1</sub> =2.63) 1) LiNHBH <sub>2</sub> .NH <sub>3</sub>  (-H <sub>B</sub> =4.47) 2) LiNH <sub>2</sub> BHNH <sub>3</sub>  (-H <sub>N2</sub> =3.18) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>2</sub>	LiNHBH <sub>2</sub> .NH <sub>3</sub> (-H <sub>B</sub> =4.52) 1) LiNHBH.NH <sub>3</sub>  (-H <sub>N1</sub> =5.19) 2)LiNHBH <sub>2</sub> .NH <sub>2</sub>  (-H <sub>N2</sub> =4.80) 3) LiNBH.NH <sub>3</sub>	LiNHBH.NH <sub>3</sub> (-H <sub>N2</sub> =2.57) 1) LiNBH.NH <sub>3</sub>  (-H <sub>B</sub> =2.92) 2) LiBNH.NH <sub>3</sub>  (-H <sub>N1</sub> =4.48) 3)LiNHBH.NH <sub>2</sub>	LiNBH.NH <sub>3</sub> (-H <sub>B</sub> =4.97) 1) LiNB.NH <sub>3</sub>  (-H <sub>N2</sub> =5.15) 2)LiNBH.NH <sub>2</sub>	LiNB.NH <sub>3</sub> (-H <sub>N2</sub> =6.51) LiNB.NH <sub>2</sub>	LiNB.NH <sub>2</sub> (-H <sub>N2</sub> =3.81) LiNB.NH	LiNB.NH (-H <sub>N2</sub> =4.24)			
LiBH <sub>2</sub> BH <sub>3</sub> (-H <sub>B</sub> =3.68) (bridged H) 1)LiBH <sub>2</sub> BH <sub>2</sub> (-H <sub>B1</sub> =4.53) 2)LiBHBH <sub>3</sub>	LiBH <sub>2</sub> BH <sub>2</sub> (-H <sub>B1</sub> =5.24) 1) LiBHBH <sub>2</sub>  (-H <sub>B1</sub> =5.12)	LiBH <sub>2</sub> BH (-H <sub>B1</sub> =4.19) 1)LiBHBH  (-H <sub>B2</sub> =4.76)	LiBHBH (-H <sub>B</sub> =5.83) LiBBH	LiBBH (-H <sub>B2</sub> =5.30) LiBB						

	2)LiBH <sub>2</sub> BH	2)LiBH <sub>2</sub> B								
LiNH <sub>2</sub> BH <sub>3</sub> .BH <sub>3</sub> (-H <sub>B</sub> =4.60) LiNH <sub>2</sub> BH <sub>2</sub> .BH <sub>3</sub> LiNH <sub>2</sub> BH <sub>3</sub> .BH <sub>2</sub> (-H <sub>N</sub> =4.85) LiNHBH <sub>3</sub> .BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>2</sub> .BH <sub>3</sub> (-H <sub>N</sub> =2.53) 1) LiNHBH <sub>2</sub> .BH <sub>3</sub> (-H <sub>B</sub> =5.55) 2) LiNH <sub>2</sub> BH <sub>2</sub> .BH <sub>2</sub>	LiNHBH <sub>2</sub> .BH <sub>3</sub> (-H <sub>B2</sub> =4.56) 1) LiNHBH <sub>2</sub> .BH <sub>2</sub> (-H <sub>N</sub> =4.94) 2)LiNBH <sub>2</sub> BH <sub>3</sub> (-H <sub>B1</sub> =4.66) LiNHBH.BH <sub>3</sub>	LiNHBH <sub>2</sub> .BH <sub>2</sub> (-H <sub>N</sub> =3.04) LiNBH <sub>2</sub> .BH <sub>2</sub> (-H <sub>B1</sub> =4.38) LiNHBH.BH <sub>2</sub>	LiNBH <sub>2</sub> .BH <sub>2</sub> (-H <sub>B1</sub> =4.41) 1)LiNBH.BH <sub>2</sub>	LiNBH.BH <sub>2</sub> (-H <sub>B1</sub> =3.36)  (-H <sub>B2</sub> =5.34) 2) LiNBH.BH	LiNBBH <sub>2</sub> (-H <sub>B2</sub> =4.33) LiNBBH	LiNBBH (-H <sub>B2</sub> =3.21)			
LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>3</sub> (-H <sub>B</sub> =3.71) (bridged H) 1)LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>2</sub> (-H <sub>N</sub> =5.18) 2)LiBH <sub>2</sub> NH <sub>2</sub> .BH <sub>3</sub>	LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>2</sub> (-H <sub>N</sub> =5.12) 1)LiBH <sub>2</sub> NH <sub>2</sub> .BH <sub>2</sub> (-H <sub>B1,2</sub> =5.19) 2)LiBHNH <sub>3</sub> .BH <sub>2</sub> 3)LiBH <sub>2</sub> NH <sub>3</sub> .BH	LiBH <sub>2</sub> NH <sub>2</sub> .BH <sub>2</sub> (-H <sub>B1</sub> =3.57) 1)LiBHNH <sub>2</sub> .BH <sub>2</sub> (-H <sub>N</sub> =4.58) 2) LiBH <sub>2</sub> NH.BH <sub>2</sub> (-H <sub>B2</sub> =4.49) 3) LiBH <sub>2</sub> NH <sub>2</sub> .BH	LiBHNH <sub>2</sub> .BH <sub>2</sub> (-H <sub>B2</sub> =4.66) 1) LiBHNH <sub>2</sub> .BH (-H <sub>B1</sub> =5.01) 2) LiBNH <sub>2</sub> .BH <sub>2</sub>  (-H <sub>N</sub> =3.51) 3) LiBHNH.BH <sub>2</sub>	LiBHNH.BH <sub>2</sub> (-H <sub>B1</sub> =4.50) 1)LiBNH.BH <sub>2</sub> (-H <sub>N</sub> =4.60) 2) LiBHN.BH <sub>2</sub> (-H <sub>B2</sub> =4.40) 3) LiBHNH.BH	LiBHNH.BH (-H <sub>B1</sub> =3.14) 1)LiBNH.BH (-H <sub>B2</sub> =5.41) 2)LiBHNH.B (-H <sub>N</sub> =4.47) LiBHN.BH	LiBNH.BH (-H <sub>N</sub> =3.84) 1)LiBNBH (-H <sub>B2</sub> =4.69) LiBNH.B	LiBNBH (-H <sub>B2</sub> =4.34) LiBNB			
LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub> BH <sub>3</sub> (-H <sub>B2</sub> =4.43)1) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> BH <sub>3</sub> (-H <sub>N2</sub> =5.18) 2)LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>2</sub> BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> BH <sub>3</sub> <sup>3</sup> (-H <sub>N2</sub> =2.34) 1)LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>2</sub> BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>2</sub> BH <sub>3</sub> (-H <sub>B1</sub> =4.58) 1) LiNH <sub>2</sub> BH.NH <sub>2</sub> BH <sub>3</sub> (-H <sub>B2</sub> =4.60)	LiNH <sub>2</sub> BH.NH <sub>2</sub> BH <sub>3</sub> (-H <sub>N2</sub> =2.99) 1) LiNH <sub>2</sub> BH.NHBH <sub>3</sub> (-H <sub>B1</sub> =5.19)	LiNH <sub>2</sub> BH.NHBH <sub>3</sub> (-H <sub>B2</sub> =4.46) 1) LiNH <sub>2</sub> BH.NHBH <sub>2</sub> (-H <sub>N2</sub> =4.92)	LiNH <sub>2</sub> BH.NHBH <sub>2</sub> (-H <sub>B1</sub> =4.19) 1) LiNH <sub>2</sub> B.NHBH <sub>2</sub> (-H <sub>N1</sub> =3.55)	LiNH <sub>2</sub> BHNBH <sub>2</sub> (-H <sub>B2</sub> =4.44) 1)LiNH <sub>2</sub> BHNBH (-H <sub>B1</sub> =4.62) 2)	LiNH <sub>2</sub> BHNBH (-H <sub>N1</sub> =4.54) 1) LiNHBH.NBH (-H <sub>B1</sub> =5.35)	LiNH <sub>2</sub> BH.NB (-H <sub>B1</sub> =4.48) 1) LiNH <sub>2</sub> B.NB	LiNH <sub>2</sub> B.NB (-H <sub>N1</sub> =3.50) LiNHB.NB	LiNHB.NB (-H <sub>N1</sub> =5.46) LiNB.NB

	(-H <sub>B2</sub> =5.07) 2) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> BH <sub>2</sub>	2) LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>2</sub> BH <sub>2</sub> (-H <sub>N2</sub> =4.73) 3)LiNH <sub>2</sub> BH <sub>2</sub> .NHBH <sub>3</sub> (-H <sub>N1</sub> =4.72) LiNHBH <sub>2</sub> .NH <sub>2</sub> BH <sub>3</sub>	2) LiNH <sub>2</sub> BH.NH <sub>2</sub> BH <sub>2</sub>	2)LiNH <sub>2</sub> BH.NBH <sub>3</sub> (-H <sub>B1</sub> =4.78) 3)LiNH <sub>2</sub> BH.NBH <sub>3</sub> (-H <sub>N1</sub> =5.39) 4) LiNHBH.NHBH <sub>3</sub>	2)LiNHBH.NHBH <sub>2</sub> (-H <sub>B2</sub> =3.93) LiNH <sub>2</sub> BHNHBH (-H <sub>N2</sub> =2.76) 3)LiNH <sub>2</sub> BHNBH <sub>2</sub>	LiNHBHNBH <sub>2</sub> (-H <sub>N1</sub> =5.52)	2)LiNH <sub>2</sub> BNBH (-H <sub>B2</sub> =2.96) LiNH <sub>2</sub> BH.NB	(-H <sub>N1</sub> =5.46)  LiNHBH.NB		
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Table (S7): NBO Chart of all the molecules

Series	Compounds	NBO Charges		
		N	B	Li
NH <sub>3</sub>	NH <sub>3</sub>	-1.049		
	NH <sub>2</sub>	-0.553		

	NH	-0.215		
	N	0.000		
BH <sub>3</sub>	BH <sub>3</sub>	0.335		
	BH <sub>2</sub>	0.329		
	BH	0.356		
	B	0.000		
NH <sub>3</sub> BH <sub>3</sub>	NH <sub>3</sub> BH <sub>3</sub>	-0.837	-0.151	
	NH <sub>2</sub> BH <sub>3</sub>	-0.692	-0.176	
	NH <sub>2</sub> BH <sub>2</sub>	-0.996	0.442	
	NH <sub>2</sub> BH	-1.089	0.458	
	NHBH	-1.006	0.664	
	BNH	-1.148	0.741	
	BN	-0.853	0.853	
LiNH <sub>2</sub>	LiNH <sub>2</sub>	-1.559		0.886
	LiNH	-1.146		0.857
	LiN	-0.846		0.846
LiBH <sub>2</sub>	LiBH <sub>2</sub>	-0.370		0.645
	LiBH	-0.458		0.671
	LiB		-0.366	0.366
LiNH <sub>2</sub> BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>3</sub>	-1.139	-0.189	0.837
	LiNH <sub>2</sub> BH <sub>2</sub>	-1.170	0.131	0.418
	LiNHBH <sub>2</sub>	-1.227	0.280	0.849

	LiNHBH	-1.321	0.325	0.718
	LiNBH	-1.402	0.559	0.934
	LiNB	-1.559	0.629	0.930
LiBH <sub>2</sub> NH <sub>3</sub>	LiBH <sub>2</sub> NH <sub>3</sub>	-0.862	-0.569	0.416
	LiBH <sub>2</sub> NH <sub>2</sub>	-0.981	0.271	0.113
LiNH <sub>2</sub> NH <sub>3</sub>	LiNH <sub>2</sub> NH <sub>3</sub>	N <sub>1</sub> =-1.507 N <sub>2</sub> =-1.085		0.794
	LiNH <sub>2</sub> NH <sub>2</sub>	N <sub>1</sub> =N <sub>2</sub> = -1.045		0.788
	LiNHNH <sub>2</sub>	N <sub>1</sub> =-1.015 N <sub>2</sub> =-0.770		0.811
	LiNHNH	N <sub>1</sub> =-0.735 N <sub>2</sub> =-0.734		0.834
	LiNNH	N <sub>1</sub> =-0.470 N <sub>2</sub> =-0.560		0.753
	LiNN	N <sub>1</sub> =-0.355 N <sub>2</sub> =-0.354		0.709
LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub>	N <sub>1</sub> =-1.111 N <sub>2</sub> =-1.060	-0.179	0.714
	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub>	N <sub>1</sub> =-1.141 N <sub>2</sub> =-1.101	0.053	0.481
	LiNHBH <sub>2</sub> .NH <sub>3</sub>	N <sub>1</sub> =-1.193	0.281	0.738



		$N_2 = -1.067$		
	$\text{LiNHBH}_3 \cdot \text{NH}_3$	$N_1 = -1.274$ $N_2 = -1.078$	0.336	0.630
	$\text{LiNBH}_3 \cdot \text{NH}_3$	$N_1 = -1.327$ $N_2 = -1.091$	0.521	0.849
	$\text{LiNB} \cdot \text{NH}_3$	$N_1 = -1.486$ $N_2 = -1.092$	0.592	0.843
	$\text{LiNB} \cdot \text{NH}_2$	$N_1 = -0.909$ $N_2 = -0.691$	0.110	0.760
	$\text{LiNB} \cdot \text{NH}$	$N_1 = -0.748$ $N_2 = -0.523$	0.141	0.793
	$\text{LiNBN}$	$N_1 = -0.638$ $N_2 = -0.229$	0.099	0.768
$\text{LiBH}_2\text{NH}_3 \cdot \text{NH}_3$	$\text{LiBH}_2\text{NH}_3 \cdot \text{NH}_3$	$N_1 = -0.863$ $N_2 = -1.096$	-0.559	0.404
	$\text{LiBH}_2\text{NH}_2 \cdot \text{NH}_3$	$N_1 = -0.996$ $N_2 = -1.104$	0.142	0.269
$\text{LiBH}_2\text{BH}_3$	$\text{LiBH}_2\text{BH}_3$		$B_1 = -0.370$ $B_2 = -0.402$	0.838
	$\text{LiBH}_2\text{BH}_2$		$B_1 = -0.217$ $B_2 = -0.218$	0.811
	$\text{LiBH}_2\text{BH}$		$B_1 = -0.117$ $B_2 = -0.874$	0.826

	LiBHBH		B <sub>1</sub> =-0.338 B <sub>2</sub> =-0.337	0.808
	LiBBH		B <sub>1</sub> =0.035 B <sub>2</sub> =-0.682	0.771
	LiBB		B <sub>1</sub> =-0.103 B <sub>2</sub> =-0.995	0.892
LiNH <sub>2</sub> BH <sub>3</sub> .BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>3</sub> .BH <sub>3</sub>	-0.882	B <sub>1</sub> =-0.172 B <sub>2</sub> =-0.172	0.783
	LiNH <sub>2</sub> BH <sub>2</sub> .BH <sub>3</sub>	-0.931	B <sub>1</sub> =-0.061 B <sub>2</sub> =-0.171	0.729
	LiNHBH <sub>2</sub> .BH <sub>3</sub>	-0.998	B <sub>1</sub> =0.346 B <sub>2</sub> =-0.192	0.817
	LiNHBH <sub>2</sub> .BH <sub>2</sub>	-1.024	B <sub>1</sub> =-0.091 B <sub>2</sub> =0.092	0.768
	LiNBH <sub>2</sub> .BH <sub>2</sub>	-1.155	B <sub>1</sub> =0.290 B <sub>2</sub> =0.413	0.874
	LiNBH.BH <sub>2</sub>	-1.142	B <sub>1</sub> =0.338 B <sub>2</sub> =0.279	0.761
	LiNB.BH <sub>2</sub>	-1.331	B <sub>1</sub> =0.305 B <sub>2</sub> =0.474	0.771

	LiNB.BH	-1.364	B <sub>1</sub> =0.285 B <sub>2</sub> =0.480	0.675
	LiNBB	-1.449	B <sub>1</sub> =0.380 B <sub>2</sub> =0.380	0.689
LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>3</sub>	LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>3</sub>	-1.063	B <sub>1</sub> =-0.387 B <sub>2</sub> =-0.388	0.741
	LiBH <sub>2</sub> NH <sub>3</sub> .BH <sub>2</sub>	-01.060	B <sub>1</sub> =-0.206 B <sub>2</sub> =-0.206	0.682
	LiBH <sub>2</sub> NH <sub>2</sub> .BH <sub>2</sub>	-1.141	B <sub>1</sub> =-0.063 B <sub>2</sub> =-0.538	0.837
	LiBHNH <sub>2</sub> .BH <sub>2</sub>	-1.130	B <sub>1</sub> =0.144 B <sub>2</sub> =-0.322	0.799
	LiBHNH.BH <sub>2</sub>	-1.146	B <sub>1</sub> =-0.130 B <sub>2</sub> =0.158	0.840
	LiBHNH.BH	-1.128	B <sub>1</sub> =0.044 B <sub>2</sub> =0.173	0.759
	LiBNH.BH	-1.136	B <sub>1</sub> =0.226 B <sub>2</sub> =-0.164	0.786
LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub> BH <sub>3</sub>	LiNH <sub>2</sub> BH <sub>3</sub> .NH <sub>3</sub> BH <sub>3</sub>	N <sub>1</sub> =-1.117 N <sub>2</sub> =-0.865	B <sub>1</sub> =-0.165 B <sub>2</sub> =-0.176	0.728
	LiNH <sub>2</sub> BH <sub>2</sub> .NH <sub>3</sub> BH <sub>3</sub>	N <sub>1</sub> =-1.138	B <sub>1</sub> =-0.079	0.678

		$N_2 = -0.900$	$B_2 = -0.185$	
	$\text{LiNH}_2\text{BH}_2 \cdot \text{NH}_2\text{BH}_3$	$N_1 = -1.149$ $N_2 = -895$	$B_1 = 0.245$ $B_2 = -0.167$	0.814
	$\text{LiNH}_2\text{BH} \cdot \text{NH}_2\text{BH}_3$	$N_1 = -1.172$ $N_2 = -0.935$	$B_1 = 0.236$ $B_2 = -0.175$	0.792
	$\text{LiNH}_2\text{BH} \cdot \text{NHBH}_3$	$N_1 = -1.133$ $N_2 = -1.044$	$B_1 = -0.176$ $B_2 = 0.698$	0.846
	$\text{LiNH}_2\text{BH} \cdot \text{NHBH}_2$	$N_1 = -1.030$ $N_2 = -1.090$	$B_1 = -0.023$ $B_2 = 0.631$	0.595
	$\text{LiNH}_2\text{BH} \cdot \text{NBH}_2$	$N_1 = -1.246$ $N_2 = -1.038$	$B_1 = 0.303$ $B_2 = 0.738$	0.859
	$\text{LiNH}_2\text{BH} \cdot \text{NBH}$	$N_1 = -1.209$ $N_2 = -1.033$	$B_1 = 0.331$ $B_2 = 0.630$	0.692
	$\text{LiNH}_2\text{BH} \cdot \text{NB}$	$N_1 = -1.326$ $N_2 = -1.010$	$B_1 = 0.255$ $B_2 = 0.694$	0.755

	LiNH <sub>2</sub> B.NB	N <sub>1</sub> =-1.357 N <sub>2</sub> =-1.074	B <sub>1</sub> =0.249 B <sub>2</sub> =0.753	0.648
	LiNHB.NB	N <sub>1</sub> =-1.416 N <sub>2</sub> =-1.051	B <sub>1</sub> =0.262 B <sub>2</sub> =0.970	0.830
	LiNB.NB	N <sub>1</sub> =-1.369 N <sub>2</sub> =-0.602	B <sub>1</sub> =0.336 B <sub>2</sub> =0.779	0.837