Determination of the molecular structure of amorphous $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ through infrared spectroscopic and computational studies

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ABSTRACT

The infrared absorption spectrum of amorphous $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ was measured in the mid-infrared region between 600 and 3300 cm^{-1} . In the frequency range corresponding to B-H stretching vibrations, the observation of absorptions due to the movements of Mg-H-B bridging hydrides provides evidence of direct bond between octahydrotriborate ions and magnesium. Starting from this configuration, DFT and ab-initio calculations at the MP2, B3LYP and B97D level were utilized in order to find the lowest energy geometry of the $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ complex. The results of all the computational studies indicate that the interaction of Mg with the $[\text{B}_3\text{H}_8]^-$ ions entails two B-Mg and two B-H-Mg bonds. The calculated infrared absorptions closely reproduce the experimental spectrum. Moreover, calculations provide evidence of the stabilization of the THF solvate of $\text{Mg}(\text{B}_3\text{H}_8)_2$ and indicate that the THF complex has a greater stabilization energy than dialkyl ethers complexes by ~25 kJ/mol.

KEYWORDS

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Infrared spectroscopy; DTF calculations; ab-initio calculations; structure; amorphous; solvation energy

1. INTRODUCTION

Mg(BH₄)₂ has attracted recent interest due to its high hydrogen content (~14.9 wt%) and the measured low enthalpy of dehydrogenation (-57±5 kJ/mol H₂). [1- 3] Experimentally, the direct hydrogenation from MgB₂ requires extreme conditions (T> 400 °C, p~900 bar). [4] However, reversible dehydrogenation has been demonstrated to occur under milder conditions (T~ 250 °C, p~120 bar) [5] according to following the equation:

which corresponds to a reversible capacity of ~2.5%. More recently, it has been reported that even milder conditions (50 bar H₂, 200 °C, 2h) can be used for hydrogenation of a 1:2 molar mixture of Mg(B₃H₈)₂(THF)₂ (where THF = tetrahydrofuran) and MgH₂ to Mg(BH₄)₂. [6]

To the best of our knowledge, there were no reports of the synthesis of Mg(B₃H₈)₂(THF)₂ prior to the study of Ref. 6 and the complex has not been structurally characterized.

However, the amorphous nature of this complex prevents the use of diffraction for the determination of its structure. The NMR measurements clearly indicate the presence of the octahydrotriborate [B₃H₈]⁻ ion in the sample as well as the presence of a THF adduct. [6]

However, more information about the interaction of the THF molecules and the [B₃H₈]⁻ ions with Mg would greatly enhance the understanding of this compound and provide valuable insight into the mechanism of its reversible hydrogenation. These structural details can be revealed by a combination of infrared spectroscopy and DFT calculations.

The infrared spectra of molecules containing BH bonds has been extensively studied and a systematic attribution of BH stretching bands to different molecular structures has been reported.[7] In particular, Kim et al. [8] pointed out that magnesium and $[\text{B}_3\text{H}_8]^-$ compounds containing ether solvates can have a ionic or a non-ionic character. In the first case, Mg is coordinated only to the ether molecules (for example, in $\text{Mg}(\text{THF})_6(\text{B}_3\text{H}_8)_2$ and in $\text{Mg}(\text{diglyme})_2(\text{B}_3\text{H}_8)_2$) and in the infrared spectrum one observes only the absorption bands due to bridging B-H-B (around 2100 cm^{-1}) and to terminal B-H (above 2400 cm^{-1}) stretching. On the other hand, $\text{Mg}(\text{B}_3\text{H}_8)_2$, $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Et}_2\text{O})_2$ and $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Me}_2\text{O})_2$ are molecular species with a direct bond of Mg to the octahydrotriborate ions and they display an additional stretching band around 2300 cm^{-1} due to the bridging Mg-H-B movements.[8] Moreover, $[\text{B}_3\text{H}_8]^-$ ions can be coordinated to an atom, M, by means of one or more B-M chemical bonds, with additional H-M bonds. For example, in $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Et}_2\text{O})_2$ and $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Me}_2\text{O})_2$ there are two B-Mg and two H-Mg bonds for each octahydrotriborate ion.[8] However, in $\text{Ag}(\text{CNB}_3\text{H}_7)_2^-$ there is one B-N and two H-N bonds.[9] In the crystal structure of NaB_3H_8 , each Na is surrounded by four octahydrotriborate anions: for two of them, Na is closer to two B atoms, while for the other $[\text{B}_3\text{H}_8]^-$ ions, Na is closer to a single B.[9, 10] Finally, the low temperature solid phase of $(\text{CO})_3\text{MnB}_3\text{H}_8$ contains three Mn-H-B bridging hydrides, one bridge bond for each boron atom.[11]

Serrar et al. showed that ab-initio calculations at the MP2 level of theory and of density functional theory methods at the B3LYP level can be applied to the study of the structure of the isolated $[\text{B}_3\text{H}_8]^-$ ion and the ClCuB_3B_8 complex.[12, 13] These authors found that in the complex the most stable structure is that in which two boron atoms are bound to the Cu atom via two B-H-Cu hydrogen bonds (one bridge bond for each B atom). Guided by these previous studies, we have utilized a combination of infrared spectroscopy measurements, ab-initio and DFT calculations in order to determine the most stable

structure of the $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ molecule. We have found that Mg is directly linked to each octahydrotriborate ion by two B-Mg and two bridge B-H-Mg bonds.

2. MATERIALS AND METHODS

$\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ (THF = tetrahydrofuran) was prepared by the addition of $\text{BH}_3 \cdot \text{THF}$ to Mg/Hg amalgam, using the procedure reported in Ref. 6.

In recent works about borohydrides, the KBr technique has been avoided because BH_4 can exchange with Br, due to their similar ionic radii.[14] In the present case, the radius of B_3H_8 is much larger and should not give this problem. However, in order to exclude spurious effects we performed infrared spectroscopy measurements in two different configurations: in transmission geometry using a pure pellet (without KBr or other salts) or by means of an Attenuated Total Reflectance accessory (ATR) on the hydride powders. The first method gives saturated bands in the BH stretching region, but provides very well defined spectra below 1700 cm^{-1} , where the intensity of bands is much lower. On the other hand, the second method is well suited in the BH stretching region. It must be noted, however, that ATR displays the same features obtained in the case of the pure pellet below 1700 cm^{-1} , but with a lower quality of the measurement. Therefore, in the following we will report data obtained by ATR between 1800 and 3300 cm^{-1} and by transmission measurements on the pure pellet in the frequency range 600 - 1700 cm^{-1} . In this framework, infrared spectroscopy measurements below 1800 cm^{-1} were performed at room temperature by means of a Agilent Cary 660 spectrometer equipped with a ceramic source, a MCT detector and a KBr beamsplitter. A small amount of the sample was pressed in a dye in order to obtain a self standing pellet. As $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ is sensitive to air, the pellet was placed in a vacuum tight cell during measurements. Above 1800 cm^{-1} data were collected by means of a Bruker Alpha spectrometer equipped with an ATR

accessory. In all cases, all handling of the sample was performed in a glove bag fluxed by an inert argon atmosphere to avoid contaminations [15, 16]. All absorption spectra were collected with a spectral resolution of 2 cm^{-1} .

3. CALCULATION

Preliminary geometries of the isolated $[\text{B}_3\text{H}_8]^-$, THF and $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ were obtained by means of the Avogadro software using the universal force field energy minimization routine.[17, 18] Ab-initio and DFT calculations were performed starting from those geometries by means of the Firefly package.[19, 20] In all cases we used the 6-31G** basis set. The wxMacMolPlt software was used to visualize the molecular geometries and vibrations [21]. After calculation of the infrared active vibrations, the IR spectrum was simulated by summing Lorentzian curves centered at each calculated IR vibration frequency with a fixed 10 cm^{-1} peak width.

4. RESULTS AND DISCUSSION

4.1 The isolated $[\text{B}_3\text{H}_8]^-$ ion

Preliminary ab-initio and DFT calculations were performed on isolated $[\text{B}_3\text{H}_8]^-$ and THF, in order to verify that the geometries agree with those found experimentally: i.e. in THF the four C atoms reside in the same plane, whilst the O atom is located outside; for $[\text{B}_3\text{H}_8]^-$ two H atoms reside in the plane of the three B atoms (see Fig. S1 of the Supplementing Material). In the present work we optimize geometries with the following theories: MP2, B3LYP and B97D. Table S1 reports the main bond lengths found in this study. One can note a good agreement with those reported in a previous DFT study [12, 13] and those

found experimentally [22, 23].

Fig. 1 Comparison of the calculated infrared absorption of isolated $[B_3H_8]^-$ at the MP2, B3LYP and B97-D level of theories.

The infrared active vibrations of isolated $[B_3H_8]^-$ were calculated with the various theories and the simulated absorbance curves are reported in Fig. 1. All the three used theories provide evidence that in the region of the B-H stretching, one finds two less intense bands below 2400 cm^{-1} (band A and B) which are due to bridging B-H-B movements and two structured bands (C and D) in the frequency region between 2450 and 2700 cm^{-1} , which can be attributed to terminal B-H stretching. The spectra calculated by the different theories look similar, but are almost rigidly shifted toward lower frequency in the following order: MP2, B3LYP and B97D. All theories are able to give the main features of the

infrared spectrum of isolated $[\text{B}_3\text{H}_8]^-$ ion. It should be noted that in most samples [8] the experimental bands A and B are centered between 2050 and 2150 cm^{-1} , whilst bands C and D are found between 2400 and 2600 cm^{-1} . In Fig. 1 it seems that the frequencies calculated by the theory B97-D are in closer agreement with the experimental values. One must keep in mind, however, that experimental infrared spectra of molecules in which the octahydrotriborate ion is linked to an atom display additional bands in the frequency range between lines A-B and C-D.[8]

The IR active vibrations of isolated THF are above this spectral range. In fact, experimentally THF possesses intense IR bands around 2975, 2960, 2891, 1460, 1450 cm^{-1} and below.[24] Computationally those bands are shifted toward higher energies by about 100 cm^{-1} .

4.2 The $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ complex

Fig. 2 displays the experimental absorption spectrum of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ in the region of B-H stretching bands.

First of all, we did not observe OH stretching bands above 3000 cm^{-1} , which would indicate contamination from water; the structured absorption band reported in Fig. 2 between 2800 and 3100 cm^{-1} is due to the vibrations of the THF molecules of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$.

Moreover, previous NMR measurements [6] indicated that no other borohydride except B_3H_8 should be present. Both observations suggest the occurrence of a pure sample, without important contaminations.

In Fig. 2 one can note the presence of two weaker bands around 2069 and 2115 cm^{-1} and two strong bands around 2385 and 2432 cm^{-1} . Moreover, a large and structured band around 2300 cm^{-1} is clearly visible. This band was attributed to the stretching vibrations of the B-H-Mg in similar compounds.[8] Therefore, our compound has a molecular structure

with Mg directly linked to the octahydrotriborate ion. Very recently it has been shown that also the newly synthesized $\text{LiB}_3\text{H}_8(\text{THF})$ complex shows infrared absorption bands due to Li-H-B bridging bonds.[25] However, computational work should be used to identify the most stable structure of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$, i.e. whether Mg is linked to one, two or three B atoms and how many H bridge bonds are present.

Fig. 2 Comparison of the measured infrared absorption with calculations for η^1 - $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ and η^2 - $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ at the MP2, B3LYP and B97-D level of theories.

We explored these various geometries for the $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ complex. Similar systems in which a metal atom was linked to the B_3H_8 ion and some other organic molecules, such

as diethyl ether, methyl ether, cyclopentadienyl or THF were used as a starting point.[8,9] In the compounds containing THF, tetrahydrofuran is attached to the metal atom through the O atom.[8] Therefore, we started the optimizing procedure from a geometry with the two THF molecules pointing towards Mg by means of the O atom. B₃H₈ groups can be attached to Mg by means of one, two or three B-Mg chemical bonds (η^1 , η^2 and η^3 structures).[8, 9] We could not obtain any stable structure in which there are three boron atom for each B₃H₈ group linked to Mg atom. Indeed, during the attempted optimization procedure the octahydrotriborate broke up. Table 1 reports the energies of the optimized geometries of η^1 and η^2 Mg(B₃H₈)₂(THF)₂ at the MP2, B97D and B3LYP level of theory, while Fig. 3 displays the optimized geometries at the MP2 level.

Fig. 3 Optimized geometries for η^1 - $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ (on the right) and η^2 -
 $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ (on the left) at the MP2 level.

The data presented in Table 1 shows that independently of the theory used for calculations, the η^2 structure has always a lower energy than the η^1 and, therefore, the former is the most thermodynamically stable. Table 2 reports the length of the main bonds found for $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ at the different levels of theory. The B-H bond lengths are generally overestimated, but there is a general good agreement between calculated and experimental B-B, Mg-B, Mg-H and Mg-O bond lengths measured in similar systems.

Table 1 Energies of different optimized geometric structures of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ (in Hartree) at various theory levels. In all cases the basis set is fixed at the 6-31G** level.

	η^1	η^2
MP2	-821.2082062	-821.2220657
B97D	-823.3737212	-823.3898445
B3LYP	-823.8287362	-823.8345862

Table 2 Main bond length of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ at different levels of theory and comparison with the experimental values reported for $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Et}_2\text{O})_2$, $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Me}_2\text{O})_2$ and $\text{Cp}_2\text{Mg}(\text{THF})$ obtained by means of XRD measurements [8].

	η^2 this study MP2	η^2 this study B3LYP	η^2 this study B97D	Exp $\text{Mg}(\text{B}_3\text{H}_8)_2$ $(\text{Et}_2\text{O})_2$ [8]	Exp $\text{Mg}(\text{B}_3\text{H}_8)_2$ $(\text{Me}_2\text{O})_2$ [8]	Exp $\text{Cp}_2\text{Mg}(\text{THF})$ [8]
B1-H4	1.19-1.22	1.20	1.21	1.12-1.17	1.08-1.14	

B1-H10	1.24-1.25	1.25-1.26	1.26-1.27	1.02	1.10-1.17	
B2-H10	1.41-1.44	1.42-1.45	1.45-1.49	1.43	1.38-1.45	
B2-H6	1.19	1.20	1.21	1.02	1.11-1.17	
B1-B2	1.81	1.81-1.82	1.81-1.82	1.795	1.780-1.803	
B1-B3	1.79	1.79	1.81	1.779	1.777-1.795	
B3-Mg	2.51	2.52	2.58	2.575	2.559	
B1-Mg	2.54	2.55	2.62	2.591	2.572	
H5-Mg	1.95	1.97	1.96	1.99	1.91	
H6-Mg	1.97	1.99	1.99	2.01	1.98	
Mg-O	2.10	2.12	2.10			2.093
H5-B1	1.22	1.22-1.23	1.23-1.24	1.17	1.14-1.19	

To confirm that the compound has an η^2 structure, we calculated the infrared absorption spectrum of both η^1 - $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ and η^2 - $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ at the three theory levels (MP2, B3LYP and B97-D). The calculated absorptions are seen in Figure 2. The spectra obtained by means of different theories for each structure are very similar, except that they are shifted toward higher frequencies as one proceeds from B97-D, to B3LYP and finally to MP2. For the η^1 structure the frequencies of the bridged B-H-B vibrations are usually underestimated; moreover, for B3LYP and MP2 the B-H-B stretching frequencies are so close that they could not be resolved and would appear as a single band in an infrared spectrum. Generally, for each level of computation, the calculated absorbance of the η^2 structure is much less structured than that of the η^1 structure and more closely resembles the experimental absorption spectrum. These features and the results of the minimization of energy suggest that the actual structure of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ is the η^2 .

Table 3 displays the infrared active stretching vibrations frequencies found at the MP2, B3LYP and B97-D level for η^2 -Mg(B₃H₈)₂(THF)₂. The vibration frequencies calculated at the B97-D level of theory are the closer to the experimental ones. However, it can be noted, that despite the succession of infrared lines is correctly described by calculations, all experimental frequencies are lower than those calculated by all models. Possibly this fact can be due to the anharmonicity of the B-H bonds, similarly to the case of alkali borohydrides containing BH₄ ions.[26]

Table 3 Calculated infrared vibration frequencies and intensities of η^2 -Mg(B₃H₈)₂(THF)₂ at different level of theory in the region of the B-H stretching vibrations and comparison with the frequencies of the experimental bands.

attribution	MP2		B3LYP		B97D		Exp
	ω (cm ⁻¹)	I (km/mol)	ω (cm ⁻¹)	I (km/mol)	ω (cm ⁻¹)	I (km/mol)	ω (cm ⁻¹)
Bridged B-H-B stretching	2336	31.4	2259	21.1	2214	23.3	2069
	2337	23.7	2259	40.2	2217	28.9	2115
	2372	37.7	2295	43.8	2260	39.3	
	2372	25.5	2298	42.7	2260	35.3	
Bridged Mg-H-B stretching	2470	48.2	2374	59.2	2327	64.2	2280
	2484	343.4	2390	505.2	2344	460.5	2325
	2492	307.5	2400	249.5	2352	251.0	
	2507	181.0	2421	123.8	2373	187.9	
Terminal	2648	125.1	2572	145.6	2542	58.8	2383
	2649	71.7	2574	142.9	2542	45.9	2432

B-H stretching	2676	28.9	2576	41.0	2552	237.2	
	2677	30.5	2577	62.8	2553	125.4	
	2686	215.0	2588	179.4	2561	44.4	
	2689	23.1	2591	28.0	2562	53.7	
	2729	240.8	2645	161.9	2597	180.4	
	2730	22.0	2647	91.2	2599	112.8	

Finally Figure 4 displays the typical movements occurring in the three types of stretching vibrations: bridged B-H-B, bridged Mg-H-B and terminal B-H.

Fig. 4 Atomic displacements corresponding to selected vibrations calculated at the B97-D level, representing B-H-B bridging, Mg-H-B bridging and terminal B-H stretching movements.

The investigation of the infrared spectrum of the $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ compound was extended to lower frequencies. Fig. 5 reports the experimental absorption spectrum between 600 and 1700 cm^{-1} . Well defined peaks are visible around 678, 707, 846, 868, 922, 966, 1010, 1040, 1138, 1180, 1250, 1297, 1315, 1348, 1456 cm^{-1} , while a broad band extends up to $\sim 1600\text{ cm}^{-1}$. We did not observe the band centered around 1630 cm^{-1} , due to possible water contamination. There is a general good agreement of the calculated and experimental bands below 1200 cm^{-1} . Above this frequency the experimental spectrum becomes less well defined and a comparison with calculations is more difficult, possibly because of the amorphous nature of the compound, which broadens the absorption bands. This behavior is different from that of other hydrides, like for example NH_3BH_3 , which due to their crystalline structure display very well defined absorption bands in the whole infrared range.[27]

Fig. 5 Comparison of the experimental and calculated absorption spectrum of $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$, in the frequency range between 600 and 1700 cm^{-1} .

Once the structure of the new $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ compound is proposed thanks to the previous combined computational/experimental work, one can investigate the formation energy of the complex, also in comparison with $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Et}_2\text{O})_2$ and $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{Me}_2\text{O})_2$.

We calculated the formation energy of $\text{Mg}(\text{B}_3\text{H}_8)_2\text{M}_2$ as:

$$E_{\text{form}} = E(\text{Mg}(\text{B}_3\text{H}_8)_2\text{S}_2) - E(\text{Mg}(\text{B}_3\text{H}_8)_2) - 2E(\text{S})$$

where S = THF, Me_2O or Et_2O . Magnesium octahydrotriborate has been recently reported to be an amorphous solid.[28] However, a detailed structural investigation is not available.

We minimized the energy of an hypothetical $\text{Mg}(\text{B}_3\text{H}_8)_2$ molecule, starting from the $\text{Mg}(\text{B}_3\text{H}_8)_2(\text{THF})_2$ compound and removing THF. For this purpose we adopted ab-initio

calculations at the MP2 level of theory. The stable structure of magnesium octahydrotriborate, reported in Fig. 6, shows that each B_3H_8 ion is linked to Mg by three B-Mg and three B-H-Mg bonds. Conversely both $Mg(B_3H_8)_2(Et_2O)_2$ and $Mg(B_3H_8)_2(Me_2O)_2$ show an η^2 structure (see Fig. 6), similar to that here proposed for $Mg(B_3H_8)_2(THF)_2$, in agreement with the structure proposed by Kim et al. [8] on the basis of diffraction studies.

Fig. 6 Optimized geometries of $Mg(B_3H_8)_2$, $Mg(B_3H_8)_2(Me_2O)_2$ and $Mg(B_3H_8)_2(Et_2O)_2$ at the MP2 level.

Table 4 reports the calculated energies of $Mg(B_3H_8)_2$, THF, Me_2O , Et_2O and of the three complexes $Mg(B_3H_8)_2S_2$, $S = THF$, Me_2O or Et_2O . From these values, one obtains that the

formation energies of the two ether complexes are quite similar (-199 and -203 kJ/mol for Me₂O and Et₂O), while -227 kJ/mol is calculated for Mg(B₃H₈)₂(THF)₂. THF is, therefore, the molecule more strongly bound to magnesium octahydrotriborate.

Table 4. Calculated energies of molecules or complexes at the MP2 level. All values are expressed in Hartree.

Molecule/complex	Energy (Hartree)
THF	-231.7338875
Me ₂ O	-154.5518258
Et ₂ O	-232.9264952
Mg(B ₃ H ₈) ₂	-357.6679207
Mg(B ₃ H ₈) ₂ (THF) ₂	-821.2220657
Mg(B ₃ H ₈) ₂ (Me ₂ O) ₂	-666.8475019
Mg(B ₃ H ₈) ₂ (Et ₂ O) ₂	-823.5982098

5. CONCLUSIONS

The combination of infrared spectroscopy, ab-initio (MP2) and DFT (B3LYP, B97-D) calculations have proven to be applicable methods for determination of the molecular structure of amorphous Mg(B₃H₈)₂(THF)₂. We have found that Mg is directly linked to each octahydrotriborate ion by means of two B-Mg and two bridge B-H-Mg bonds. B97-D functional seems to be the best choice to reproduce the experimental spectrum in the whole mid infrared range between 600 and 3300 cm⁻¹, even though anharmonicity of the BH stretching vibrations should be present. Moreover, calculations provide evidence of the

stabilization of the THF solvate of $\text{Mg}(\text{B}_3\text{H}_8)_2$ and indicate that the THF complex has greater stabilization energy than the dialkyl ethers complexes by ~ 25 kJ/mol.

ACKNOWLEDGEMENTS

PN and CJ acknowledge the support of the US Department of Energy, Office of Energy Efficiency and Renewable Energy.

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