Sequential bond energy, binding energy, and structures of Be$^+$ · (H$_2$)$_{1–3}$ complexes

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Abstract. The binding energy and structures of the Be cations with H$_2$ molecules are studied theoretically at the MP2/aug-cc-pVTZ method level. The structures of the Be$^+$ · (H$_2$)$_{1–3}$ complexes are determined. A tee and a vee-shaped structure are obtained for mono- and di-ligated complexes. Trigonal prism geometry is discovered in the tri-ligated complex. The sequential bond energies of the Be$^+$ · (H$_2$)$_{1–3}$ complexes are also examined. The variation in the trend in sequential bond dissociation energies that have been observed may be due to variations in the electrostatic interaction energies, electronic charge transfer, and repulsive forces between the H$_2$ ligands in these complexes.

Keywords. MP2; Beryllium ions; H$_2$ molecule; Sequential bond dissociation energy; NBO analysis.

1. Introduction

A long time ago, the ion-ligand complex formation between cations or anions and H$_2$ molecules was studied and investigated.$^{1,2}$ The most important issues of these studies are understanding the interactions of hydrogen molecules with ions and other technical reasons, such as hydrogen storage and purification.$^{3–5}$ The ability of the materials used to attract or adsorb (physisorbed) the H$_2$ molecules and their stabilities under acceptable conditions are two major factors influencing the hydrogen storage process. In addition, these materials allow the kinetics of hydrogen ad- and desorption very fast and highly reversible since no structural change occurs in the framework of these systems.$^6$ Therefore, it is preferable to investigate how H$_2$ molecules interact with one another and with materials located on them.$^7$ One of the goals of this research is to investigate the capacity of beryllium ions in terms of how much they attract H$_2$ molecules and their stabilities. On a variety of surfaces, the impact of ions on the amount of H$_2$ stored has also been investigated experimentally and theoretically.$^{8–10}$ The use of liquid H$_2$ as a clean and renewable energy source is the final goal of these studies. However, the interaction potential of hydrogen molecules is still not completely determined (except for its ground rotational state) because of quantum rotational effects, particularly in liquid and solid phases.$^{11,12}$ Many studies have been performed to understand the behavior of these molecules in liquid and solid phases and the nature of the interaction between H$_2$ molecules and different types of ions in the last 30 years.

Beryllium is a very hazardous element that is carcinogenic and the root cause of the possibly fatal chronic beryllium disease (CBD), which is worth mentioning here.$^{13}$ A successful cleanup process must be developed in order to guarantee workplace safety and lessen environmental contamination. Since studying the interactions between Be ions and other ligands in these circumstances is exceedingly dangerous, there have never been any experimental data on Be$^+$ ions binding with H$_2$ molecules. The complexation of cations/anions with H$_2$ molecules is formed due to electrostatic forces such as charge ion-quadrupole and ion-induced dipole interactions, besides induction interactions. The predominant electrostatic interaction has largely determined the structure of these complexes, as published in previous years.$^{14,15}$ Many theoretical studies on the interaction of anions or cations with H$_2$ molecules have formed new cationic and anionic clusters.$^{16,17}$ Many studies have been performed on the interaction of beryllium cations with H$_2$ molecules. The structure of a weak complex [Be · H$_2$]$^+$ is determined

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theoretically on the basis of the MP4/6-31G* level calculations. These results have shown that the Be$^+$ ion is directed toward the midpoint of the H$_2$ molecule at a distance of 1.751 Å, in a T-shaped structure. These findings were consistent with previous theoretical studies, despite the fact that the symmetry of the [Be$^+$·H$_2$]$^+$ in its ground-state structure is still a subject of continuous debate. Hinze anticipated that symmetry breakdown would occur in the two Be–H bonds and his claim was qualitatively justified by means of molecular orbital (MO) reasoning. In other theoretical studies, the equilibrium structure with C$_{2v}$ symmetry was predicted. The potential energy surface was also examined using SCF calculations, which showed that the dissociation energy of the Be$^+$·H$_2$ complex is 5.19 kcal mol$^{-1}$. Recently, the potential energy surface of the Be$^+$·H$_2$ the complex has been revisited again using high levels of ab initio methods. The potential energy surface of the Be$^+$·H$_2$ complex has been studied using corrected, coupled-cluster (CC), and multi-reference configuration interaction (MRCI) methods. These calculations showed that the Be$^+$·H$_2$ complex has a global minimum of a T-shaped structure with a C$_{2v}$ symmetry and a transition state of linear structure with a D$_{xh}$ symmetry. The binding energy between the Be$^+$ ion and H$_2$ molecule in the T-shaped structure was found to be 5.8 kcal mol$^{-1}$. In that direction, the interaction of the Be$^+$ ion with H$_2$ and D$_2$ molecules has been investigated theoretically. The structure and binding energy of Be$^+$·H$_2$ and Be$^+$·D$_2$ were determined at the CCSD(T)/aug-cc-pVQZ level of theory. In addition, a 3D ground state potential energy surface is also obtained. The Be$^+$ ion forms a complex with H$_2$ in a T-shaped structure at a distance of 1.776 Å between them. However, no research has ever been done on the interaction forces that the Be$^+$ cation experiences when interacting with several H$_2$ molecules, and neither theoretical nor experimental information regarding these complexes and their structures have been published.

In this paper, we hope to add to what has already been published by characterizing the interaction between beryllium cations and several hydrogen molecules. The structures and binding energies of the Be$^+$·(H$_2$)$_n$ complexes ($n = 1–3$) are determined. Furthermore, the sequential bond energies of these complexes are also studied and determined. The electrostatic potential of these complexes is also under investigation. Our results are compared with the available published data.

2. Computational details

All calculations were conducted using the Gaussian 03 software package, in which the parameters of the optimized geometry and electronic energy of all complexes are carried out at the level of the MP2 method. In this work, the aug-cc-pVTZ basis set was used for all atoms in these complexes. The basic set applied consists of polarized and diffuse functions which are suitable for our calculations for these complexes.

The minimum and saddle point states, as well as the reaction paths extending down from a transition state structure on the potential energy surface were determined using the intrinsic reaction coordinates (IRC) and vibration frequency testing. Then, the zero-point energy (ZPE) for each stationary point was computed at T = 298 K.

The difference between the electronic energy, including zero-point energy, of the complex and the total electronic and zero-point energies of the uncomplexed cation and diatomic molecules was used to calculate the binding energy. Using the full counterpoise method, the resulting energy value was then corrected for basis set superposition error (BSSE). The sequential bond dissociation energies of the Be$^+$·(H$_2$)$_n$ complexes were computed using the following equation for the minimum states at different structures:

$$Be^+ \cdot (H_2)_n \rightarrow Be^+ \cdot (H_2)_{n-1} + H_2 \quad (n : 1–3) \quad (1)$$

The interaction’s Wiberg bond index (WBI) was used to investigate the strength of the attraction forces between the Beryllium cation and the hydrogen molecules. In addition, the bond order (BO) of the H$_2$ molecule within the complex was also calculated to understand the nature of complexation. This can be obtained based on NBO analysis calculations using the MP2/aug-cc-pVTZ method.

To provide a more realistic depiction of the interaction forces in these complexes, the successive bond dissociation energies for the Be$^+$·(H$_2$)$_{1,3}$ complexes are determined. The fluctuation in the electrostatic interaction energies could explain the computed bond dissociation energy trend. Thus, the electrostatic interaction of a fully charged Be$^+$ cation with a non-polar H$_2$ molecule can be divided into ion-quadrupole interactions and ion-induced dipole interactions. These contributions are computed based on the Be$^+$·H$_2$ geometry coordinates presented in Figure 1, using the formula below.
\[ E_{\text{elec.}} = \frac{Q_{\text{Be}} \cdot \Theta_{H_2}}{4\pi\varepsilon_0 R^3} \cdot (3 \cdot \cos^2 \theta - 1) + \frac{Q_{\text{Be}}^2 \cdot 2_{H_2}}{8\pi\varepsilon_0 R^4} \]  

(2)

where the former and the latter represent the ion-quadrupole and ion-induced dipole interactions, respectively. \( Q \) is the calculated NBO point charge at the Be atomic site, \( \Theta \) is the \( H_2 \) molecule’s quadrupole moment, \( +0.6177 \) \( \text{D} \), \( 29 \) and \( \varepsilon \) is the polarizability of molecular \( H_2 \), \( 0.799 \) \( \text{Å}^3 \). \( R \) represents the magnitude of the vector connecting the mass center of the \( H_2 \) molecule and the position of the \( \text{Be}^+ \) ion in space. \( \theta \) is the angle restricted between the molecular axis of \( H_2 \) and \( \vec{R} \). \( \varepsilon_0 \) denotes the vacuum’s permittivity.

3. Results and Discussion

3.1 The \( \text{Be}^+ \cdot H_2 \) complex

At the UMP2/aug-cc-pVTZ technique level, the interaction between a \( \text{Be}^+ \) ion and an \( H_2 \) molecule is examined and analyzed. The complex has a minimal state, as shown in Figure 2, where the \( \text{Be}^+ \) cation is pointed at the \( H_2 \) molecule’s bond center at a distance of 1.803 Å, forming a T-shaped structure. The complex also possesses a transition state where the \( \text{Be}^+ \) cation is oriented toward one of the \( H_2 \) terminals at a distance of 2.228 Å from the \( \text{Be}^+ \) ion to the \( H_2 \) mass center, forming a linear shape. In addition, the one-dimensional potential energy surface (PES) for the complex’s T-shaped structure has been investigated at various polar angles \( \theta \) and is presented in Figure 3. The interaction energy was estimated as a function of the distance, \( z \), between them. This interaction energy included ZPE and BSSE corrections. According to these estimates, which support the IRC results, the complex has a tee-shaped structure with a binding energy of about 6.2 kcal/mol.

The optimized geometrical parameters of the \( \text{Be}^+ \cdot H_2 \) complex in its different states are listed in Table 1 and compared with other published data. Our calculated results agree well with those published, as may be seen in Table 1. The T-shaped structure of the \( [\text{Be} \cdot H_2]^+ \) exhibits a stretching frequency of 4181.8 cm\(^{-1}\), shifted to red by 334.6 cm\(^{-1}\) with respect to that of a free \( H_2 \) molecule. Our findings agreed well with 4082 cm\(^{-1}\) (red-shifted by 320 cm\(^{-1}\) compared with that of free molecular \( H_2 \)) calculated on the basis of the CCSD(T)/aug-cc-pVQZ method.\(^{22}\) The vibration frequency test shows that the linear structure, with symmetry of a \( D_{\text{sh}} \), represents a transition state with an imaginary frequency of 588.4i cm\(^{-1}\) plus two other frequencies of 381.8 cm\(^{-1}\)
and 4230.5 cm\(^{-1}\) for \(\text{H} - \text{H}\) stretching. These results are calculated using the UMP2/aug-cc-pVTZ level of theory.

We already know that the \(\text{H}_2\) molecule has a positive quadrupole moment,\(^{29}\) which causes a permanent positive charge distribution to be positioned on the hydrogen atomic sites (terminals) and a negative charge distribution to be concentrated at the mid-bond between the two atomic sites. These observations support the T-shaped structure, which is formed as a minimum due to strong attraction interactions between the \(\text{Be}^+\) ionic site and the negative charge present in the center of the \(\text{H}_2\) molecule. The linear shape indicates a transition state since the \(\text{Be}^+\) ion forms a repulsive electrostatic connection with either of the \(\text{H}_2\) molecule’s terminals. Thus, the NBO analysis of the atomic charge distribution and Wiberg bond index (WBI) values for molecular \(\text{H}_2\) and the \(\text{Be}^+\cdot\text{H}_2\) complex in different configurations is studied using the UMP2/aug-cc-pVTZ method, as presented in Figure 4. These results reveal that the variations in the positive charge of the \(\text{Be}^+\) ion in both linear and T-shaped structures are insignificant. In the T-shaped structure, the electrons of the sigma bond of \(\text{H}_2\) are unaffected by the \(\text{Be}^+\) ion since the two hydrogen atoms have almost zero atomic charge distribution (\(\approx 0.035\)). Note here that the bond order (BO) of \(\text{H}_2\) is slightly affected and still equals \(\approx 0.94\). This is consistent with an elongation in the bond length of \(\text{H}_2\) by 0.039 Å upon complexation with the \(\text{Be}^+\) cation. It seems that the electronic charge of \(\text{H}_2\) has been redistributed between \(r_1s\) and \(r_3s\). The electrons in the \(\sigma\) bond are polarized in a transition state linear configuration, where the electrons partially migrate toward the H atom closest to the \(\text{Be}^+\) ion, creating a negative charge on the H atomic site closest to the ion while the second hydrogen exhibits a positive charge, as shown in Figure 4. However, the bond order of \(\text{H}_2\) is slightly changed to become \(\approx 0.94\), even though the \(\text{Be}^+\) ionic charge is still unchanged. This situation indicates the electrostatic nature of interaction forces within the \(\text{Be}^+\cdot\text{H}_2\) complex. WBI values show that the strength of the interaction in a T-shaped minimum structure is almost twice as strong as that of a transition state linear structure.

As shown in Table 2, the binding energy of the \(\text{Be}^+\cdot\text{H}_2\) complex in its T-shaped structure is calculated using the UMP2/aug-cc-pVTZ method and found to exhibit a binding energy of 6.2 kcal/mol\(^{-1}\). Our result agrees well and is consistent with 7.6 and 5.8 kcal/mol\(^{-1}\) that were calculated on the basis of the MRCI/ANO-RCC/aug-cc-pVQZ\(^{20}\) and the CCSD(T)/aug-cc-pVQZ\(^{22}\) methods, respectively. However, the binding energies calculated for the T-shaped structure using the UMP2/aug-cc-pVTZ and CCSD(T)/aug-cc-pVQZ methods are \(\sim 2.4\) greater than those calculated using the MP4/6-31G* method.\(^{16}\) This is due to the level of basis set applied in the MP4 method.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Method</th>
<th>Basis set</th>
<th>(r_1^{\text{Be-H}_2}) (Å)</th>
<th>(r_1^{\text{H-H}}) (Å)</th>
<th>(\theta^\circ)</th>
</tr>
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<tbody>
<tr>
<td>(\text{Be}^+\cdot\text{H}_2) complex</td>
<td>UMP2</td>
<td>aug-cc-pVDZ</td>
<td>1.801</td>
<td>0.777</td>
<td>90.0</td>
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<tr>
<td></td>
<td></td>
<td>aug-cc-pVTZ</td>
<td>1.803</td>
<td>0.762</td>
<td>90.0</td>
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<tr>
<td></td>
<td>HF</td>
<td>6-31G(d)(^a)</td>
<td>1.751</td>
<td>0.746</td>
<td>90.0</td>
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<tr>
<td></td>
<td>IC-MRCI</td>
<td>ANO-RCC/aug-cc-pVQZ(^b)</td>
<td>1.816</td>
<td>0.761</td>
<td>90.0</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)</td>
<td>Aug-cc-pVQZ(^c)</td>
<td>1.776</td>
<td>0.768</td>
<td>90.0</td>
</tr>
<tr>
<td>Linear TS</td>
<td>UMP2</td>
<td>aug-cc-pVDZ</td>
<td>2.224</td>
<td>0.767</td>
<td>180.0</td>
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<tr>
<td></td>
<td></td>
<td>aug-cc-pVTZ</td>
<td>2.228</td>
<td>0.752</td>
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<td></td>
<td>IC-MRCI</td>
<td>ANO-RCC/aug-cc-pVQZ(^b)</td>
<td>2.152</td>
<td>0.761</td>
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<tr>
<td></td>
<td>CCSD(T)</td>
<td>aug-cc-pVQZ(^c)</td>
<td>2.153</td>
<td>0.761</td>
<td>180.0</td>
</tr>
<tr>
<td>(\text{H}_2)</td>
<td>MP2</td>
<td>aug-cc-pVTZ</td>
<td>-</td>
<td>0.738</td>
<td>-</td>
</tr>
</tbody>
</table>

\(^a\)Represent the distance between the \(\text{Be}^+\) ion and the midpoint of \(\text{H}_2\) bond. \(^b\)Taken from ref.\(^{16}\) \(^c\)Taken from ref.\(^{20}\)
3.2 The $\text{Be}^+(\text{H}_2)_2$ and $\text{Be}^+(\text{H}_2)_3$ complexes

The optimized geometrical parameters of the $\text{Be}^+(\text{H}_2)_2$ and $\text{Be}^+(\text{H}_2)_3$ complexes, in their doublet state ($^2A_1$), are presented in Figure 5. The IRC test and vibration frequency calculations show that each complex exhibits one minimum and one transition state structure. The minimum state generally exhibits a structure in which the $\text{Be}^+$ ion is directed vertically along the middle of each H$_2$ bond in the complex. The transition state (results not shown) exhibits a sub-linear structure where the $\text{Be}^+$ ion is directed toward either of the H$_2$ terminals with an angle of 180.0°.

The binding energy ($\text{BE}$) of the beryllium cations bonded with more than one H$_2$ molecule is calculated using the UMP2/aug-cc-pVTZ method. These results are listed in Table 2. Our calculations show that the tri-ligated complex, $\text{Be}^+(\text{H}_2)_3$, has the largest binding energy among all of these complexes presented in this study. The binding energy was found to be increased with H$_2$ molecules. To explain the obtained BE trend, $\text{Be}^+\cdot\text{H}_2 < \text{Be}^+\cdot(\text{H}_2)_2 < \text{Be}^+\cdot(\text{H}_2)_3$, the NBO analysis of these complexes was performed, and the results are shown in Figure 6. The WBI values show that the tri-ligated complex exhibits the strongest interaction between the $\text{Be}^+$ ion and the H$_2$ molecule. Furthermore, the obtained WBI exhibits the same trend as the one obtained for the binding energy, BE, of these complexes. We found that the separations between the $\text{Be}^+$ ion and the H$_2$ molecules for the mono-ligated to tri-ligated complexes follow the same order as that obtained for the BE of these complexes. As expected, the binding energy, BE, should increase as the $\text{Be}^+$···H$_2$ separation decreases. The $\text{Be}^+\cdot(\text{H}_2)_3$ complex, in particular, has the shortest distance with the $\text{Be}^+$ ion, with a value of 1.442 Å.

One of the important factors affecting the binding energy is the distance between the H$_2$ ligands inside the complex. Our NBO calculations show that the di-ligated complex has the shortest separation between the centers of mass of H$_2$ molecules in the complex.
This will create a larger intra-repulsive interaction among H$_2$ ligands and hence decrease the stability of the di-ligated complex. This conclusion supports increasing the BE as the complex transitions from a di-ligated complex to a tri-ligated complex.

3.3 The molecular orbital diagram

The molecular orbital (MO) diagram of these complexes is examined using the NBO analysis approach in order to find an explanation for the variations in the length of the H$_2$ bond and the charges present on the beryllium cationic site in these complexes. Using the UMP2/aug-cc-pVTZ approach, the NBO analysis of the electronic population of these complexes was computed. These results are presented in Figure 7. First of all, the mono-ligated complex exhibits a negligible electronic charge transfer, $\sigma_{1s} \rightarrow 2s, 2p$, of 0.07. The electronic charge transfer, $\sigma_{1s} \rightarrow 2s, 2p$, is increased with the H$_2$ molecules in these complexes. This becomes very important in the tri-ligated complex. Briefly, the amount of electronic charge transfer per one H$_2$ molecule toward the Be$^+$ ion in these complexes follows the order: Be$^+ \cdot H_2, 0.07, <Be^+ \cdot (H_2)_2, 0.11, <Be^+ \cdot (H_2)_3, 0.22$. These results also show that the tri-ligated complex has the largest value of electronic charge transfer, $\sigma_{1s} \rightarrow 2s, 2p$, which is consistent with the findings of the BE values and the shortest Be$\cdots$H$_2$ distance among these complexes consists of more than a single H$_2$ molecule. The MO diagram shows that the elongation in the H$_2$ bond length, particularly in the tri-ligated complexes, is around 0.077 Å due to electronic charge transfer from the hydrogen molecule toward the Be$^+$ ion. The elongation in the molecular H$_2$ is around 0.03 Å for the mono- and di-ligated complexes. The bond order (BO) of H$_2$ in these complexes was found to follow the order: Be$^+ \cdot H_2 (0.94) <Be^+ \cdot (H_2)_2 (0.96) <Be^+ \cdot (H_2)_3 (1.11)$. It seems the amount of electronic charge transfer is reflected in the BO values of molecular H$_2$ within these complexes.

3.4 Sequential bond dissociation energies of Be$^+ \cdot (H_2)_n (n = 1 - 3)$

The sequential bond dissociation energies (SBDE) of these complexes were calculated based on Eq. (1) using the UMP2/aug-cc-pVTZ method. These results show that the tri-ligated complex has the largest value of electronic charge transfer, $\sigma_{1s} \rightarrow 2s, 2p$, which is consistent with the findings of the BE values and the shortest Be$\cdots$H$_2$ distance among these complexes consists of more than a single H$_2$ molecule. The MO diagram shows that the elongation in the H$_2$ bond length, particularly in the tri-ligated complexes, is around 0.077 Å due to electronic charge transfer from the hydrogen molecule toward the Be$^+$ ion. The elongation in the molecular H$_2$ is around 0.03 Å for the mono- and di-ligated complexes. The bond order (BO) of H$_2$ in these complexes was found to follow the order: Be$^+ \cdot H_2 (0.94) <Be^+ \cdot (H_2)_2 (0.96) <Be^+ \cdot (H_2)_3 (1.11)$. It seems the amount of electronic charge transfer is reflected in the BO values of molecular H$_2$ within these complexes.

Figure 7. NBO analysis results of the MO diagram of the Be$^+ \cdot (H_2)_n (n = 1 - 3)$ complexes calculated based on the UMP2/aug-cc-pVTZ method. The numbers above each molecular H$_2$ and Be$^+$ ion level represent their populations. It is worth noting that the electronic population of H$_2$ in the Be$^+ \cdot (H_2)_2 (2 - 3)$ complexes represents a single H$_2$ molecule in the complex.
are listed in Table 3. Our results show that the sequential bond dissociation energies start to decrease from mono- to di-ligated complexes as a result of decreasing the \( \text{Be} \cdots \text{H}_2 \) distances, which has a greater effect than that decreasing the charges located on the ionic site. The tri-ligated complex has the largest SBDE value among all of these complexes. This can be attributed to the fact that the largest value of the electronic charge transfer, \( \sigma_1s \rightarrow 2s, 2p \), occurred in that complex and hence decreased largely the separation between the metal ion and \( \text{H}_2 \) ligand by approximately 22%. This means that the SBDEs of the complexes adopt the following order: \( \text{Be}^+ \cdot \text{H}_2 > \text{Be}^+ \cdot (\text{H}_2)_2 < \text{Be}^+ \cdot (\text{H}_2)_3 \). To explain the obtained SBDE trend, the electrostatic energy, based on the NBO results, was calculated using Eqn. 2, and is presented in Figure 8. The electrostatic results of these complexes were compared with their SBDE values. As shown in Figure 8, the variation in the electrostatic values relatively matches the obtained trend in the SBDE values of these complexes. We thought that the electrostatic energy and electronic charge transfer, besides the separations between the \( \text{Be}^+ \) ion and the \( \text{H}_2 \) molecules, were the forces behind the variation in the BE and SBDE values. It is worth mentioning the separations between the \( \text{Be}^+ \) ion and \( \text{H}_2 \) ligands and the charges present on atomic sites in these complexes, which produce a different trend, especially as it transitions from di- to tri-ligated complexes, as seen in Figure 8.

4. Conclusions

We have investigated the nature of interactions, structures, and binding energies of the \( \text{Be}^+ \cdot (\text{H}_2)_n (n = 1 \text{–} 3) \) complexes by the UMP2 method. These results are found to agree well with those reported from previous studies, where available. A tee-shaped structure is obtained for a mono-ligated complex, whereas a vee-shaped structure is obtained for a di-ligated complex. For tri-ligated complexes, trigonal prism geometry is formed. According to the UMP2 calculations, the values of SBDE followed a certain pattern, with the tri-ligated complex exhibiting the highest value among all of these complexes. The repulsive forces generated among the \( \text{H}_2 \) ligands in these complexes, electronic charge transfer, and fluctuations in the electrostatic energies, which are primarily brought on by the ion-quadrupole and the ion-induced dipole interaction energies, are what lead to the predicted SBDE trend in these ion complexes.

**Table 3.** Sequential bond dissociation energies (SBDE) of the \( \text{Be}^+ \cdot (\text{H}_2)_n (n = 1 \text{–} 3) \) complexes calculated at the UMP2/aug-cc-PVTZ method. The units are in kcal mol\(^{-1}\).

<table>
<thead>
<tr>
<th>Complex</th>
<th>SBDE</th>
<th>BSSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Be}^+ \cdot \text{H}_2 )</td>
<td>6.2</td>
<td>0.084</td>
</tr>
<tr>
<td>( \text{Be}^+ \cdot (\text{H}_2)_2 )</td>
<td>4.8</td>
<td>0.172</td>
</tr>
<tr>
<td>( \text{Be}^+ \cdot (\text{H}_2)_3 )</td>
<td>16.3</td>
<td>0.364</td>
</tr>
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</table>

**Figure 8.** The SBDE and electrostatic energy for \( \text{Be}^+ \cdot (\text{H}_2)_n (n = 1 \text{–} 3) \) calculated at the level of the UMP2/aug-cc-PVTZ method.

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