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The formation of hydride bonds in cationic complexes of $n\mathrm{BeH_2}\cdots m\mathrm{X}$ with $n = 1$ or 2, $m = 1$ or 2 and $\mathrm{X} = \mathrm{Li}^+$ or Na^+

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Abstract: The optimized geometries and topological parameters of the $\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots\mathrm{Li}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots2\mathrm{Na}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Li}^+$ and $\mathrm{BeH_2}\cdots2\mathrm{Li}^+$ cationic complexes were obtained through BHandHLYP/6--31G(d,p) calculations. Besides the characterization of one or two hydride bonds formed simultaneously on the same hydride center, the analysis of the infrared spectra revealed the existence of red-shifts and blue-shifts on the BeH bonds, the effects of which are not in line with the intermolecular interaction strength determined by means of the supermolecule approach. Quantum theory of atoms in molecules (QTAIM) calculations were developed to measure the charge density concentration on the $\mathrm{H}\cdots\mathrm{Na}^+$ and $\mathrm{H}\cdots\mathrm{Li}^+$ hydride bonds. Moreover, the covalent character of these interactions, interpreted based on the ratio between the kinetic and potential electronic energies, was also examined.

Keywords: hydride bonds; infrared; QTAIM.

INTRODUCTION

Since the pioneering insights of Moore, Winmill, Lewis and Pauling, and surely without forgetting the contributions elaborated by Pimentel and McClellan,[1] over all these years, the hydrogen bond was acclaimed as the matriarchal interaction throughout the world of chemistry.[2–7] Some time ago, however, Crabtree *et al*.[8] discovered another type of interaction called the dihydrogen bond in which two hydrogen atoms interact mutually, although one of them is often attributed to a hydride bound with an alkaline earth metal. In some cases, the dihydrogen bond concept is interpreted as an inverse hydrogen bond, although at first sight this interaction might be anomalous once the contact is doubly electropositive.[9,10] In addition, the chemical literature recognizes the existence of this vanguard group of new intermolecular interactions in nature[11] as being formed

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by halogen bonds,[12] halogen–hydride bonds,[13] picanogen bonds,[14] or even beryllium bonds.[15]

Nevertheless, one of the most innovative investigations with involvement of alkaline earth metals and hydride compounds is the formation of intermolecular complexes in the configuration of cations,[16] namely as $BeH_2\cdots Li^+$, $BeH_2\cdots Na^+$ and $BeH_2\cdots Mg^{2+}$. A comparison with similar interactions must be worthwhile,[17] although knowledge of the vibration stretch modes followed by their absorption intensities in the infrared spectrum is always treated as one of the states of art upon the formation of intermolecular interactions, such as those in the $C_2H_5^+\cdots\pi$, $BeH_2\cdots HCF_3$ and $LiH\cdots HCF_3$ complexes.[18,19] In this scenario, there are two forms of analyses, namely: the identification of new vibration modes commonly called intermolecular frequency interactions ($H\cdots Na^+$ and $H\cdots Li^+$) or the frequencies of proton donors (Be–H) shifted to upward or downward values followed by decreasing, or sometimes an increasing, absorption intensities.[20–23] Regarding the main purpose of the present study, the formation of cationic systems does not occur in the sense of dihydrogen bonds[7,8] but actually of hydride bonds. Although sodium and lithium cation are not proton donors, they are considered acids whereas beryllium hydride is the basis.

In view of this, this current work was elaborated with the aim of studying the $BeH_2\cdots Na^+$ and $BeH_2\cdots Li^+$ bimolecular complexes, but not only in the light of these bimolecular configurations. Actually, it must be emphasized that trimolecular complexes formed with acids or proton acceptors in excess enlarge the horizons in any intermolecular study once the search for the most stable configuration among three entities is recognized as no easy task.[24] Thus, besides the bimolecular complexes of $BeH_2\cdots Na^+$ and $BeH_2\cdots Li^+$, the trimolecular forms represented by $BeH_2\cdots 2Na^+$ and $2BeH_2\cdots Na^+$, as well as $BeH_2\cdots 2Li^+$ and $2BeH_2\cdots Li^+$, form part of a selected group of systems in which such structures must be governed by the formation of multiple hydride interactions.

COMPUTATIONAL DETAILS

The geometries of the complexes were obtained at the BHandHLYP/6-31G(d,p) level of theory with all calculations executed by the Gaussian 03W[25] program. With the coordinates of the optimized geometries, the QTAIM modeling was developed by the AIMAll 11.05.16 suite of codes.[26]

Additional parameters and the coordinates of the optimized geometries of the $BeH_2\cdots Na^+$, $2BeH_2\cdots Na^+$, $BeH_2\cdots 2Na^+$, $BeH_2\cdots Li^+$, $2BeH_2\cdots Li^+$ and $BeH_2\cdots 2Li^+$ dihydride complexes obtained by calculations at the BhandHLYP/6-31G(d,p) level of theory given in the Supplementary material to this paper.

RESULTS AND DISCUSSION

The optimized geometries of the $BeH_2\cdots Na^+$ (**I**), $2BeH_2\cdots Na^+$ (**II**), $BeH_2\cdots 2Na^+$ (**III**), $BeH_2\cdots Li^+$ (**IV**), $2BeH_2\cdots Li^+$ (**V**) and $BeH_2\cdots 2Li^+$ (**VI**) complexes are grouped and illustrated in Fig. 1, in which the variations on the

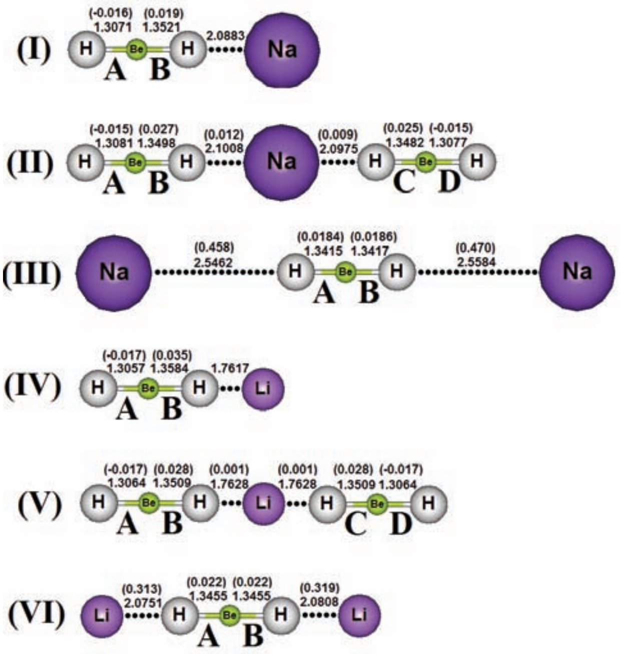

Fig. 1. Optimized geometries of the **I** ($BeH_2\cdots Na^+$), **II** ($BeH_2\cdots Na^+\cdots BeH_2$), **III** ($Na^+\cdots BeH_2\cdots Na^+$), **IV** ($BeH_2\cdots Li^+$), **V** ($BeH_2\cdots Li^+\cdots BeH_2$) and **VI** ($Li^+\cdots BeH_2\cdots Li^+$) complexes at the BHandHLYP/6-31G(d,p) level of theory. The values of the bond length of Be–H (Only in the BeH_2 monomer) is 1.3231 Å computed at the BHandHLYP/6-31G(d,p) level of theory.

bond lengths are also drawn. Due to the absence of experimental data, such as those generated by rotational spectroscopy, the intermolecular distances can be validated by the van der Waals radius of the hydrogen[27] and by the Shanoon crystal radii[28] for the lithium and sodium ions, the values of which are 1.20, 1.24, and 0.92 Å, respectively. By associating these data, the intermolecular distances of 2.44 (radii of H^+ and Na^+) and 2.12 Å (radii of H^+ and Li^+) are referential to examine the single ($H\cdots Na^+$ and $H\cdots Li^+$) and double ($Na^+\cdots H\cdots Na^+$ and $Li^+\cdots H\cdots Li^+$) hydride interactions. By taking into account the values of 2.5462 and 2.5584 Å, it can be seen that only the hydride bonds in **III** are beyond the limit of 2.44 Å. In addition, **VI** is on the intermolecular allowed threshold in that the values of 2.0751 and 2.0808 Å are shorter by 0.0449 and 0.0392 Å in comparison with the referential value of 2.12 Å. In other words, the formation of hydride bonds is valid in **III**. The hydride bond distances of the complexes are shorter than those formed by potassium and calcium when in interaction with beryllium hydride.[29]

On complexation, the structure of the BeH_2 hydride changes distinctly. For this reason, four moieties were assigned, namely A, B, C and D (see Fig. 1). The bond lengths in A and D are reduced regardless of whether a complex is bimolecular (with one BeH_2) or trimolecular (with two BeH_2). On the other hand, the bond length increases not only of B and C, but also of A and B in the complexes **III** and **VI**. Unlike all that has often been documented in the chemical literature that shorter distances followed by high interactions strengths often leads to an enlargement in the bond lengths of proton donors,[30] this systematic tendency is surely not valid here. The determination of the variations in the bond lengths was performed based on analyses of infrared spectra and the obtained values for the vibration modes are listed in Table I.

TABLE I. Values of the main infrared modes (stretch frequency and absorption intensity) of the **I**–**VI** dihydride-bonded complexes obtained from BHandHLYP/6-31G(d,p) calculations; values at the BHandHLYP/6-31G(d,p) level of theory of the stretch frequencies and absorption intensities of the Be–H oscillator are given in parenthesis; Values at the BHandHLYP/6--31G(d,p) level of theory of υ and I of the Be–H bond (BeH_2 monomer) are 2318.8 cm^{-1} and 240.5 km mol^{-1}, respectively

Mode	Dihydride complex					
	I	**II**	**III**	**IV**	**V**	**VI**
$\nu_{H\cdots 0X1}$ / cm^{-1}	249.0	198.5	48.0	385.8	234.8	159.3
$I_{H\cdots X}$ / km mol^{-1}	10.8	0.002	0.2	61.2	0.0	1.1
$\Delta\nu_{Be–H}A$ / cm^{-1}	+25.3	+21.2	–117.2	+36.2	+37.1	–282.9
	(2344.1)	(2340.0)	(2021.1)	(2120.6)	(2355.9)	(2035.9)
$I_{Be–H,c}A/I_{Be–H,m}A$	1.10	2.14	0.0	1.19	2.79	0.0
	(265.2)	(516.0)	(0.03)	(334.5)	(671.6)	(0.01)
$\Delta\nu_{Be–H}B$ / cm^{-1}	–226.9	–224.6	–117.2	–198.2	–185.1	–282.9
	(2091.9)	(2094.2)	(2021.1)	(2355.0)	(2133.7)	(2035.9)
$I_{Be–H,c}B/I_{Be–H,m}B$	1.10	1.97	0.0	1.39	2.53	0.0
	(265.6)	(474.6)	(0.03)	(287.2)	(610.1)	(0.01)
$\Delta\nu_{Be–H}C$ / cm^{-1}	–	–212.3	–	–	–172.7	–
	–	(2106.5)	–	–	(2146.1)	–
$I_{Be–H,c}C/ I_{Be–H,m}C$	–	0.16	–	–	0.0	–
	–	(38.3)	–	–	(0.0)	–
$\Delta\nu_{Be–H}D$ / cm^{-1}	–	+27.4	–	–	+44.9	–
	–	(2346.2)	–	–	(2363.7)	–
$I_{Be–H,c}D/I_{Be–H,m}D$	–	0.24	–	–	0.0	–
	–	(58.3)	–	–	(0.0)	–

The values of the new vibrational modes or hydride bond stretch frequencies are widely varied, *e.g.*, the results of 48.0 and 385.8 $cm^{–1}$ for $\nu_{H\cdots X}$ as well as 0.2 and 61.2 km $mol^{–1}$ for $I_{H\cdots X}$ in **III** and **IV**, respectively. Moreover, if the intermolecular geometry is stabilized either into a global or local minimum in the potential energy surface, the proton donor bond may be strengthened because its frequency is shifted to upward values, and in this case, the blue-shift effect is manifested. No matter if the shift is from red or blue nature,[31] these phenomena validate the bond strength profile of the proton donors. Currently, the interpretations of red shifts and blue shifts in hydrogen-bonded complexes are made if the hyperconjugation or hybridization effects are taken into account,[32] when, under these circumstances, the intermolecular system can be strong or weakly bound. Thus, in agreement with the structural analysis, the reductions in the bond lengths in the subparts of A and D were evidenced by the frequencies shifted to blue, the values of which for $\Delta\nu_{\text{Be–H,A}}$ vary from +21.2 to +37.1 cm^{-1}. Moreover, the red shifts of –117.2 and –282.9 cm^{-1} are also in excellent agreement with the increases in the Be–H bond lengths in **III** and **VI**. Regarding B and C, the red shifts are the only infrared effects manifested on their oscillators whereas in D of **II** and **V**, only blue ones are characterized. Concerning the absorption intensities, the values listed in Table I indicate unsystematic profiles. In order to understand better the synergism between the structural changes and frequency shifts in Be–H, the linear relationship between the values of the variations of the bond lengths and red shifts and blue shifts is plotted in Fig. 2.

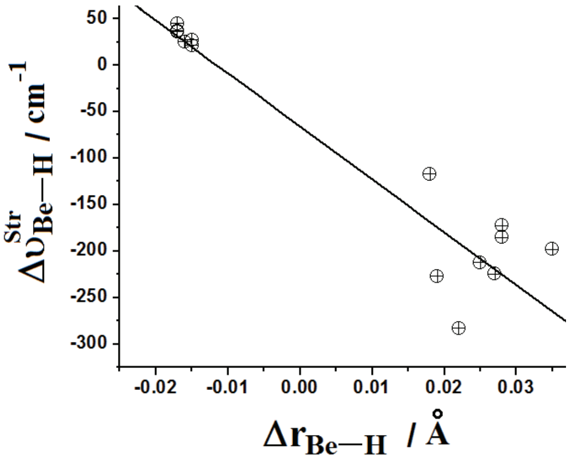

Fig. 2. Relationship between the vibrational displacement in the stretch frequencies (red- or blue-shift) *vs*. the variations on the bond length of the Be–H oscillator at the BHandHLYP/6-31G(d,p) level of theory.

The values of the hydride bond energies[33] with zero-point vibrational energy corrections (*ΔZPV*) and amendments for basis set superposition errors (*BSSE*), as well as those without adjustments are presented in Table II. The shortest bound intermolecular systems, **IV** and **V**, are those whose values of ΔE^{C} are the highest. On the other hand, the longest bound systems, in this case **III** and **VI**, have values of their interaction energies that are unreal. Not simply by the fact of extremely lengthy distances, but the *BSSE* amounts outweigh these intermolecular energies. These are intermolecular systems the stabilization of which is prejudiced by whether more than two interactions are formed. Although the enhancements on the dipole moment justify the absorption intensities of the hydride bonds of complexes **I** and **IV**, the difference between the ΔE^{C} values of –51.80 and –55.66 kJ mol^{-1} cannot be appraised by this argument. In comparison, the values of –51.80 and –75.61 kJ mol$^{–1}$ are quite close to –49.12 and –76.44 kJ mol$^{–1}$, which were obtained by Grabowski *et al.*[16] through MP2/aug-cc-pVQZ calculations. At the MP2(full)/6-31G(3df,3pd) theoretical level, a result of –51.04 kJ mol$^{–1}$ was obtained,[32] which is less stable by 0.76 kJ mol$^{–1}$ in comparison with the value of –51.80 kJ mol$^{–1}$ computed by BHandHLYP/6-31G(d,p). As can be seen, this functional theoretical level seems useful to predict the hydride bond strength or maybe any other intermolecular interaction of interest.

TABLE II. Values of the electronic parameters (dihydride bond energy with *ZPE* and *BSSE* corrections) of the **I–VI** dihydride-bonded complexes obtained from BHandHLYP/6-31G(d,p) calculations

Mode	Dihydride complex					
	I	**II**	**III**	**IV**	**V**	**VI**
ΔE / kJ mol^{-1}	–57.27	–111.11	109.63	–81.73	–156.63	98.01
ΔZPE / kJ mol^{-1}	3.40	7.33	3.48	4.39	10.07	5.85
$BSSE$ / kJ mol^{-1}	2.07	3.83	943.6	1.73	3.52	985.8
ΔE^{C} / kJ mol^{-1}	–51.80	–49.97	>10^3	–75.61	–55.66	>10^3
$\Delta\mu$ / Debye*	4.22	–0.0016	0.018	8.03	–0.0038	0.019
$\rho_{H\cdots X}$ / e a_o^{-3}	0.0158	0.0154 (0.0155)[a]	0.0068 (0.0067)[a]	0.019	0.0189 (0.0189)[a]	0.0097 (0.0096)[b]
$\nabla^2\rho_{H\cdots X}$ / a_o^{-5}	0.0772	0.0738 (0.0744)[a]	0.0189 (0.0182)[a]	0.0983	0.0975 (0.0975)[a]	0.0368 (0.0361)[b]
$G_{H\cdots X}$ / eu	0.0162	0.0155 (0.0157)[a]	0.0041 (0.0039)[a]	0.0204	0.0203 (0.0203)[a]	0.0075 (0.0074)[b]
$U_{H\cdots X}$ / eu	–0.0131	–0.0126 (–0.0127)[a]	–0.0035 (–0.0033)[a]	–0.0163	–0.0163 (–0.0163)[a]	–0.0059 (–0.0058)[b]
$H_{H\cdots X}$ / eu	0.0031	0.0029 (0.003)[a]	0.0006 (0.0006)[a]	0.0041	0.004 (–0.004)[a]	0.0016 (0.0016)[b]
$–G_{H\cdots X}/U_{H\cdots X}$	1.23	1.23 (1.23)[a]	1.17 (1.18)[a]	1.25	1.24 (1.24)[a]	1.27 (1.27)[b]

[a]Values related to the Na···H–Be–H(C/D) moiety; [b]values related to the Li···H–Be–H···Li(A/B) moiety

Nevertheless, the interaction strength is one of the main goals in intermolecular studies. Despite the quantification of the interaction strength by means of the supermolecule approach, the prediction of this parameter can be realized by analysis of topological descriptors derived from the quantum theory of atoms in molecules (QTAIM),[34] such as electronic density (ρ), Laplacian ($\nabla^2\rho$), electronic kinetic energy (G) and electronic potential energy (U), and through of them, the interaction strength can be unveiled. The values of the QTAIM parameters are also enumerated in Table I. In addition to the low electronic density, all hydride bonds were identified as closed-interactions due to the positive values of the Laplacian.[35] The QTAIM integrations were able to locate distinct electronic density

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* 1 C m = 3×10^{29} Debye

fluxes between $_{\mathrm{Be-H}}\mathrm{B}\cdots\mathrm{Na}^+$ and $\mathrm{Na}^+\cdots\mathrm{C}_{\mathrm{H-Be}}$ of **II**, $\mathrm{Na}^+\cdots\mathrm{A}_{\mathrm{H-Be}}$ and $_{\mathrm{Be-H}}\mathrm{B}\cdots\mathrm{Na}^+$ of **III**, $_{\mathrm{Be-H}}\mathrm{B}\cdots\mathrm{Li}^+$ and $\mathrm{Li}^+\cdots\mathrm{C}_{\mathrm{H-Be}}$ of **V**, and $\mathrm{Li}^+\cdots\mathrm{A}_{\mathrm{H-Be}}$ and $_{\mathrm{Be-H}}\mathrm{B}\cdots\mathrm{Li}^+$ of **VI**.

In advance, the electronic density energy or the sum of the kinetic and potential energy operators is always positive and thereby yields a low intermolecular electronic density flux, *i.e.*, U is outweighed by G. In terms of interaction strength, the rationalization between G and U would indicate a covalent character or at least partial if $-G/U < 1$,[36] or even total if $-G/U < 0.5$. Unfortunately, the values depicted in Table I suggest that all **I**–**VI** complexes are non-covalent ones.

CONCLUSIONS

A series of intermolecular complexes formed by hydride bonds were examined herein. Although the structural parameters were in good agreement with the infrared modes, the calculations of the intermolecular energies revealed unusual values, some of which were completely unacceptable. The variation of the dipole moment also fails into rationalize the interaction strength. Finally, the QTAIM method valued the existence of the hydride bonds, and albeit the intermolecular distance was very short, a covalent profile was not found, such as is well-known in other studies.[16,32]

SUPPLEMENTARY MATERIAL

Additional parameters and the coordinates of the optimized geometries of the $\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots2\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots\mathrm{Li}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Li}^+$ and $\mathrm{BeH_2}\cdots2\mathrm{Li}^+$ dihydride complexes obtained by calculations at the BhandHLYP/6-31G(d,p) level of theory are available electronically from http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

ИЗВОД

ФОРМИРАЊЕ ХИДРИДНИХ ВЕЗА У КАТЈОНСКИМ КОМПЛЕКСИМА $n\mathrm{BeH_2}\cdots m\mathrm{X}$ СА $n = 1$ ИЛИ 2, $m = 1$ ИЛИ 2 И $\mathrm{X} = \mathrm{Li}^+$ ИЛИ Na^+

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Прорачунима методама BH и HLYP/6-31G(d,p) одређене су оптимизоване геометрије и тополошки параметри за катјонске комплексе $\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots\mathrm{Li}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Na}^+$, $\mathrm{BeH_2}\cdots2\mathrm{Na}^+$, $2\mathrm{BeH_2}\cdots\mathrm{Li}^+$ и $\mathrm{BeH_2}\cdots2\mathrm{Li}^+$. Једна или две хидридне везе су се симултано градиле на истом хидридном центру. Анализа инфрацрвених спектара указује на постојање црвеног и плавог помака код двају BJ веза, што није у складу с предвиђањима на основу модела супермолекула. Помоћу QTAIM прорачуна процењена је густина наелектрисања на $\mathrm{H}\cdots\mathrm{Na}^+$ и $\mathrm{H}\cdots\mathrm{Li}^+$ хидридним везама. Разматрана је интерпретација ковалентног карактера ових интеракција на основу односа кинетичке и потенцијалне енергије.

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