

# Characteristics of beryllium bonds; a QTAIM study

K. Eskandari

Received: 17 June 2011 / Accepted: 10 January 2012 / Published online: 28 January 2012  
© Springer-Verlag 2012

**Abstract** The nature of beryllium bonds formed between  $\text{BeX}_2$  (X is H, F and Cl) and some Lewis bases have been investigated. The distribution of the Laplacian of electron density shows that there is a region of charge depletion around the Be atom, which, according to Laplacian complementary principal, can interact with a region of charge concentration of an atom in the base and form a beryllium bond. The molecular graphs of the investigated complexes indicate that beryllium in  $\text{BeH}_2$  and  $\text{BeF}_2$  can form “beryllium bonds” with O, N and P atoms but not with halogens. In addition, eight criteria based on QTAIM properties, including the values of electron density and its Laplacian at the BCP, penetration of beryllium and acceptor atom, charge, energy, volume and first atomic moment of beryllium atom, have been considered and compared with the corresponding ones in conventional hydrogen bonds. These bonds share many common features with very strong hydrogen bonds, however, some differences have also been observed.

**Keywords** Beryllium bond · Electron density · Laplacian of electron density · QTAIM · Weak interactions

## Introduction

Weak interactions play important roles in many different areas of chemistry [1–5]. Although there are a lot of types of noncovalent interactions, the hydrogen bond is, without doubt, the most important one [6–9]. In fact in a hydrogen bond, the principal role of interaction is played by the

hydrogen atom. On the other hand, the beryllium atom has some similarities to hydrogen atom; it is electropositive and, when it is covalently bonded to a more electronegative atom, has low lying empty orbitals that allow it to behave as an electron acceptor [10–14]. It seems that, Be is an element which may be regarded as a hydrogen that has a core of electrons! So, it is not surprising if Be participates in special type of interactions which share common characteristics with conventional hydrogen bonds.

Recently, Yáñez and co-workers [15] investigated the interactions between some Be containing molecules and different Lewis bases. They showed that the resulting complexes are stabilized through an interaction between the Be atom and the basic center of the base. They analyzed the bonds in these systems with three different approaches: quantum theory of atoms in molecules (QTAIM) [16], electron localization function (ELF) [17, 18] and natural bond orbital (NBO) [19]. They indicated that although these interactions are in general stronger than hydrogen bonds, they share many common features. They used the term “beryllium bond” for these interactions in order to emphasize the similarity with hydrogen bonds. In the present work, Laplacian of electron density,  $\nabla^2\rho$ , is used for some beryllium complexes, to gain a deeper understanding of the nature of these bonds. In addition, the eight QTAIM-based criteria which are proposed by Koch and Popelier [20] to detect and characterize hydrogen bonds, are tested for these beryllium bonds and compared with those in different types of hydrogen bonds.

## Computational details

Molecular geometries and their electronic wave functions were optimized at MP2/6-311+G(3df,2p) level using

K. Eskandari (✉)  
School of Chemistry, Damghan University,  
Damghan 36716-41167, Iran  
e-mail: eskandari@du.ac.ir

Gaussian 03 program [21]. Bader's quantum theory of atoms in molecules (QTAIM) [16] was used to study atomic and bond properties. Integrations over atomic basins were carried out using standard mode of AIMAll program [22]. This package was also used to draw contour and envelope maps of the negative of the Laplacian of electron density. Molecular graphs were drawn with AIM2000 [23].

The accuracy of atomic integration has been checked by the values of  $N-\Sigma N(\Omega)$  and L function,  $L(\Omega) = -\nabla^2\rho$  [24, 25]. The summations of electron atomic populations,  $N(\Omega)$ , for the molecules match the total number of electrons,  $N$ , within 0.0002 a.u. No atom was integrated with,  $L(\Omega)$ , differing from zero (the value of ideal atom delimitation [16]) by more than  $\pm 5 \times 10^{-4}$  a.u.

## Results

In the current work, the complexes formed between  $\text{BeX}_2$  (X is H, F and Cl) and some Lewis bases ( $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{H}_2\text{S}$ ,  $\text{PH}_3$ , HF, HCl and HBr) have been investigated. The calculated interaction energies for these complexes have been listed in Table 1. These values show that the strengths of the complexes span over a broad range, from 1.2 to 27.8 kcal mol<sup>-1</sup>. This energy span is comparable to the

**Table 1** Interaction energies (kcal mol<sup>-1</sup>) and QTAIM parameters (atomic units) at the beryllium bond BCP of the studied complexes

	$\Delta E + \text{BSSE}$	$\rho_b$	$L_b$	$G_b$	$V_b$	$H_b$
$\text{BeH}_2\text{—NH}_3$	-21.39	0.059	-0.342	0.093	-0.100	-0.007
$\text{BeH}_2\text{—OH}_2$	-15.66	0.056	-0.458	0.110	-0.105	0.005
$\text{BeH}_2\text{—PH}_3$	-6.09	0.036	-0.139	0.041	-0.048	-0.007
$\text{BeH}_2\text{—SH}_2$	-5.69	0.032	-0.158	0.043	-0.046	-0.003
$\text{BeH}_2\text{—FH}^a$	-4.19	—	—	—	—	—
$\text{BeH}_2\text{—ClH}$	-1.27	0.022	-0.032	0.013	-0.018	-0.005
$\text{BeH}_2\text{—BrH}^a$	-1.68	—	—	—	—	—
$\text{BeF}_2\text{—NH}_3$	-24.14	0.061	-0.331	0.093	-0.102	-0.010
$\text{BeF}_2\text{—OH}_2$	-17.40	0.056	-0.423	0.103	-0.101	0.002
$\text{BeF}_2\text{—PH}_3$	-6.84	0.035	-0.120	0.037	-0.044	-0.007
$\text{BeF}_2\text{—SH}_2$	-6.68	0.032	-0.135	0.038	-0.042	-0.004
$\text{BeF}_2\text{—FH}$	-5.96	0.033	-0.287	0.064	-0.058	0.007
$\text{BeF}_2\text{—ClH}$	-2.15	0.020	-0.056	0.017	-0.020	-0.003
$\text{BeF}_2\text{—BrH}^a$	-2.42	—	—	—	—	—
$\text{BeCl}_2\text{—NH}_3$	-27.49	0.069	-0.356	0.104	-0.118	-0.015
$\text{BeCl}_2\text{—OH}_2$	-19.13	0.065	-0.480	0.121	-0.121	-0.001
$\text{BeCl}_2\text{—PH}_3$	-9.13	0.044	-0.131	0.045	-0.058	-0.012
$\text{BeCl}_2\text{—SH}_2$	-8.10	0.040	-0.150	0.046	-0.054	-0.008
$\text{BeCl}_2\text{—FH}$	-5.10	0.040	-0.333	0.077	-0.070	0.007
$\text{BeCl}_2\text{—ClH}$	-1.56	0.028	-0.144	0.037	-0.038	-0.001
$\text{BeCl}_2\text{—BrH}$	-1.80	0.024	-0.104	0.028	-0.030	-0.002

<sup>a</sup> No BCP has been found between Be and halogen atom

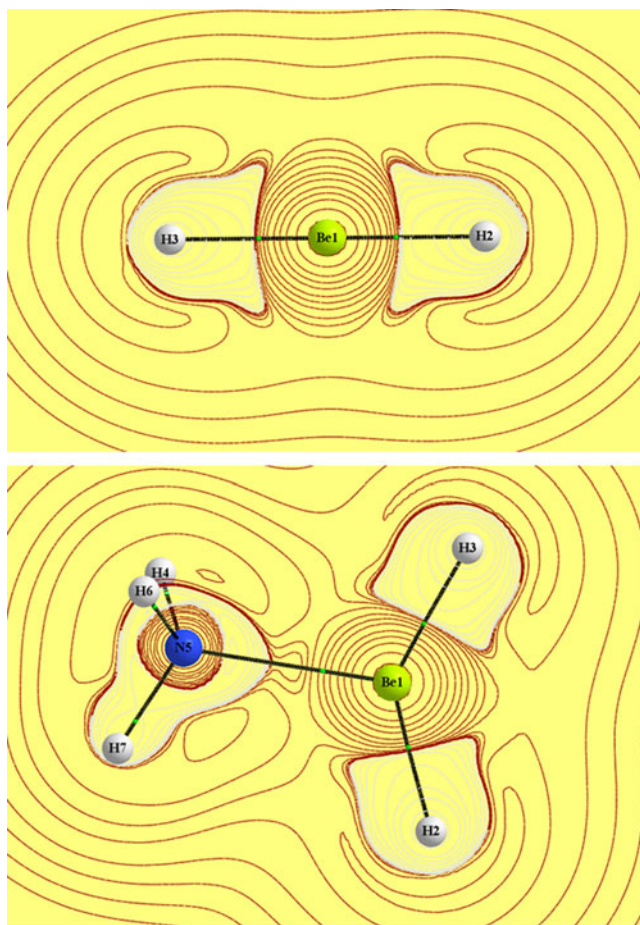
strength of hydrogen bonds. The table also shows that in complexes with same  $\text{BeX}_2$  but different base, the interaction energy is in the order  $\text{NH}_3 > \text{H}_2\text{O} > \text{PH}_3 > \text{H}_2\text{S} > \text{HF} > \text{HCl} > \text{HBr}$ . Concerning different beryllium derivatives, the order is  $\text{BeCl}_2 > \text{BeF}_2 > \text{BeH}_2$ . However, when the base is HF, HCl or HBr the order changes as  $\text{BeF}_2 > \text{BeCl}_2 > \text{BeH}_2$ .

It is well known that the QTAIM provides a powerful tool for detecting and characterizing the chemical bonds. In fact, this theory takes advantages of electron density and its derivatives as an information source to categorize and describe chemical bonds. In the following sections, electron density and its Laplacian will be used to illustrate different aspects of beryllium-base interactions.

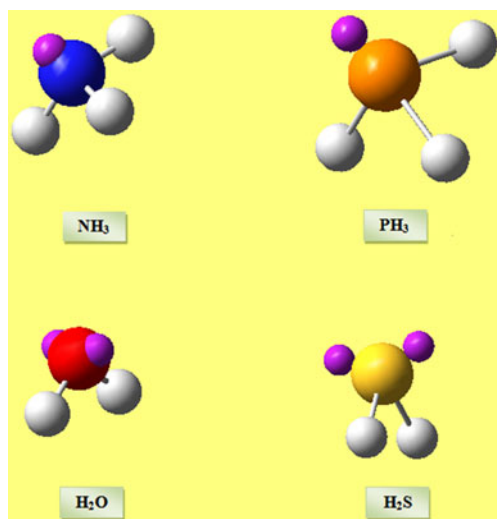
## Beryllium bond; a lump-hole interaction

In fact the Laplacian of the electron density provides a physical basis (via local statement of virial theorem) for the Lewis acid–base interactions [16, 26–28]. In essence,  $\nabla^2\rho$  measures where the electronic charge concentrated (when  $\nabla^2\rho$  is negative) and depleted (when  $\nabla^2\rho$  is positive). For easy reference, one may define L-function as the negative of Laplacian of electron density (i.e.,  $L = -\nabla^2\rho$ ) and relates the regions of charge concentration and depletions with positive and negative values of L-function, respectively. In the QTAIM point of view, the basic regions in molecules are in fact the zones where the charge is locally concentrated and conversely acidic regions are the zones where the charge is locally depleted. A Lewis acid–base interaction can be regarded as combination of a local charge concentration or a ‘lump’ in the valence shell charge concentration (VSCC) of the base with a local charge depletion or a ‘hole’ in the VSCC of the acid. Popelier called this statement “the Laplacian complementary principle” [29].

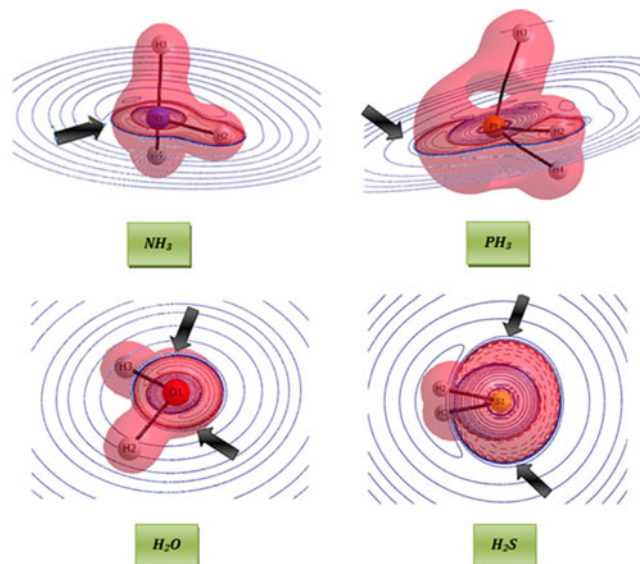
To find the regions of charge concentrations and depletions around the  $\text{BeX}_2$  molecules, their L-functions have been calculated. Figure 1 shows the contour map of the L-function for  $\text{BeH}_2$ . As can be seen, there is a region of charge depletion (hole) around the Be atom. In other words, there is an acidic region around the beryllium, which according to Laplacian complementary principle, can interact with a region of charge concentration (lump) of an atom in another molecule (base) and consequently, form a beryllium bond. As an example, the interaction between  $\text{BeH}_2$  in  $\text{NH}_3$  has been indicated in Fig. 1. The nitrogen atom in  $\text{NH}_3$  has a lump in its VSCC that interacts with the hole around the Be atom. This lump in the VSCC of nitrogen has been pointed by an arrow in contour and envelope maps of the Laplacian of electron density of  $\text{NH}_3$  in Fig. 2. Topologically, each lump in the L-function, corresponds to a (3,-3) critical point in the Laplacian of electron density (the critical points in the L-function occur where  $\nabla(\nabla^2\rho) = 0$ ) [16]. The



**Fig. 1** Contour maps of the negative Laplacian of electron density for BeH<sub>2</sub> (up) and BeH<sub>2</sub>...NH<sub>3</sub> (down). White and red lines correspond to positive and negative values respectively



**Fig. 2** The positions of non-bonded (3, -3) critical points (lumps) in the VSCC of the basic atoms



**Fig. 3** Envelope and contour maps of the Laplacian of the electron density. Arrows indicate the position of lumps in the VSCC of basic atoms

(3,-3) critical point of nitrogen atom in NH<sub>3</sub> has been shown in Fig. 3. Bonding between BeH<sub>2</sub> and PH<sub>3</sub> can be explained in the same way; there is a lump in the VSCC of phosphorus atom (Figs. 2 and 3) which interacts with the hole of beryllium. On the other hand, the oxygen and sulfur in H<sub>2</sub>O and H<sub>2</sub>S have two lumps in their VSCC (see Figs. 2 and 3) and the beryllium bond can form between one of these lumps and the hole in the VSCC of Be. The contour maps of the L-function of BeF<sub>2</sub> and BeCl<sub>2</sub> are similar to BeH<sub>2</sub>; there is a hole around the Be atom in these molecules. Again, the beryllium bonds formed between BeF<sub>2</sub> or BeCl<sub>2</sub> and bases can be regarded as lump-hole interactions. However, in these cases the region of charge concentration in the VSCC of basic atom is more polarized toward the beryllium, indicating more tendency of electron sharing between N and Be.

**Beryllium bond; is it similar to hydrogen bond?**

As stated in the introduction, Yáñez et al. [15] showed that beryllium bonds are, in general, similar to hydrogen bonds. On the other hand, Popelier and Koch [20, 29–31] used electron density as an information source to characterize hydrogen bonds. They proposed eight criteria based on the QTAIM to detect and classify hydrogen bonds. According to their results, an interaction between hydrogen and another atom can be called a hydrogen bond, if it satisfies all of these criteria. The first criterion for existence of a hydrogen bond is the presence of a bond critical point (BCP) between the hydrogen atom and the acceptor atom. The second and third criteria say that the values of electron density,  $\rho_b$ , and Laplacian of electron density,  $\nabla^2\rho_b$ , at the BCP lie,

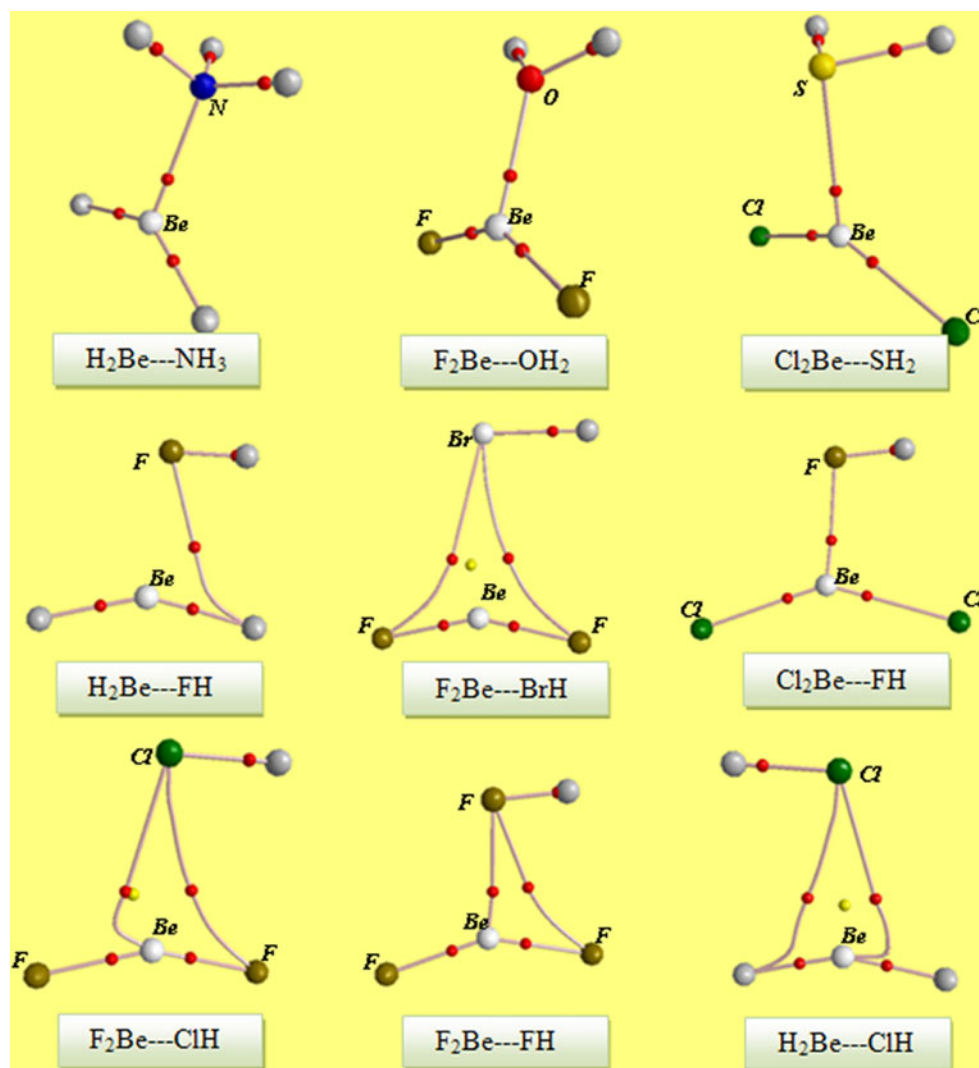
respectively, within the ranges [0.002, 0.04] a.u. and [−0.15, 0.02] a.u. The fourth criterion states that the hydrogen and the acceptor atom should penetrate each other. The fifth criterion asserts that the hydrogen atom loses charge upon formation of hydrogen bond. The sixth condition relates to energetic destabilization of hydrogen atom when a hydrogen bond is formed. And finally, the seventh and eighth criteria state that the dipolar polarization and the volume of the hydrogen atom decrease upon complex formation.

Bearing in mind that beryllium bonds have analogies with hydrogen bonds, it is reasonable to ask whether they represent similar QTAIM properties or not. So, in the next paragraphs the mentioned eight criteria is checked for beryllium bonds and compared with those of hydrogen bonds.

#### Existence of BCP

The molecular graph (MG) of  $\text{H}_2\text{Be}\cdots\text{NH}_3$  has been indicated in Fig. 4. As indicated there is a bond critical point and

**Fig. 4** The molecular graphs of the complexes. (Red dots are BCPs)



a bond path (BP) between Be and N atoms. Similar MGs have been observed for other  $\text{X}_2\text{Be}\cdots\text{NH}_3$ ,  $\text{X}_2\text{Be}\cdots\text{OH}_2$ ,  $\text{X}_2\text{Be}\cdots\text{PH}_3$ ,  $\text{X}_2\text{Be}\cdots\text{SH}_2$ ,  $\text{Cl}_2\text{Be}\cdots\text{FH}$ ,  $\text{Cl}_2\text{Be}\cdots\text{ClH}$  and  $\text{Cl}_2\text{Be}\cdots\text{BrH}$  complexes (some of these MGs presented in Fig. 4, see also supporting information of ref. [15]). In all of these cases the BCP lie somewhat closer to the beryllium atom. On the other hand, the situation is different for  $\text{X}_2\text{Be}\cdots\text{FH}$ ,  $\text{X}_2\text{Be}\cdots\text{ClH}$  and  $\text{X}_2\text{Be}\cdots\text{BrH}$  complexes (when  $\text{X}=\text{H}$  or  $\text{F}$ ). In  $\text{H}_2\text{Be}\cdots\text{FH}$  and  $\text{F}_2\text{Be}\cdots\text{BrH}$  there is no BCP and BP between Be and F, Cl or Br atoms and instead, one or two BCPs are formed between halogen in hydrogen halide and the X atom (H or F) in the  $\text{BeX}_2$  (Fig. 4). This means that beryllium bond does not form in these complexes. In the  $\text{F}_2\text{Be}\cdots\text{FH}$  and  $\text{F}_2\text{Be}\cdots\text{ClH}$ , complexes there is a halogen bond interaction in addition to beryllium-halogen interaction. It should be mentioned these results were confirmed by CCSD calculations, that is similar MGs have been observed for complexes between  $\text{X}_2\text{Be}$  and hydrogen halides when we evaluated the wavefunctions generated from CCSD/6-311+G(3df,2p) calculations.



## The charge density at the BCP

The calculated values of electron density at the BCP,  $\rho_b$ , of beryllium bonds have been listed in Table 1. It can be seen that the values of  $\rho_b$  are greater than expected values for normal hydrogen bonds and are similar to those of strong and very strong hydrogen bonds [32].

## The Laplacian of the electron density and energy density at the BCP

The values of  $\nabla^2\rho_b$  are also collected in Table 1. All of the values are negative which indicate depletion of electronic charge along the bond paths and implies an electrostatic nature for these beryllium bonds. However, the absolute values of  $\nabla^2\rho_b$  are greater than those of conventional hydrogen bonds, and are similar to strong and very strong hydrogen bonds. It has been previously shown that very strong hydrogen bonds are partially electrostatic and partially covalent [32]. This is the case for these beryllium bonds; as mentioned in Yáñez's paper [15], the negative values of electronic energy density at the BCPs,  $H_b$  (defined as  $H_b = G_b + V_b$ , in which  $G_b$  and  $V_b$  are electronic kinetics and potential energy densities [16]), proposed a partially electrostatic and partially covalent nature for beryllium bonds. The only exceptions are the bonds between beryllium and oxygen atoms in  $X_2\text{Be}\dots\text{OH}_2$  (when  $X=\text{H}$  or  $\text{F}$ ) and  $X_2\text{Be}\dots\text{FH}$  (when  $X=\text{F}$  or  $\text{Cl}$ ) complexes in which the energy densities are positive and near zero.

**Table 2** Integrated atomic properties of beryllium in the complexes and their difference with  $\text{BeX}_2$  monomers. The last column indicates the values of beryllium penetration. All of the values are in atomic units

	N(Be)	E(Be)	V(Be)	$\Delta\text{N}$	$\Delta\text{E}$	$\Delta\text{V}$	$ \Delta\text{M}_0 $	$\Delta r_{\text{Be}}$
$\text{BeH}_2\text{—NH}_3$	2.297	-14.203	15.042	0.011	0.035	-4.608	0.689	2.11
$\text{BeH}_2\text{—OH}_2$	2.287	-14.198	14.978	0.002	0.040	-4.673	0.585	2.13
$\text{BeH}_2\text{—PH}_3$	2.309	-14.214	16.615	0.024	0.024	-3.035	0.574	1.98
$\text{BeH}_2\text{—SH}_2$	2.300	-14.211	16.306	0.014	0.027	-3.344	0.530	1.98
$\text{BeH}_2\text{—FH}$	2.275	-14.197	16.015	-0.011	0.041	-3.636	0.451	—
$\text{BeH}_2\text{—ClH}$	2.285	-14.214	16.505	0.000	0.024	-3.145	0.535	—
$\text{BeH}_2\text{—BrH}$	2.286	-14.217	16.933	0.001	0.020	-2.717	0.345	—
$\text{BeF}_2\text{—NH}_3$	2.206	-14.143	10.202	0.016	0.006	-2.443	0.674	1.66
$\text{BeF}_2\text{—OH}_2$	2.197	-14.133	10.007	0.007	0.016	-2.638	0.583	1.67
$\text{BeF}_2\text{—PH}_3$	2.209	-14.140	11.079	0.019	0.010	-1.566	0.593	1.52
$\text{BeF}_2\text{—SH}_2$	2.204	-14.135	11.016	0.014	0.014	-1.628	0.555	1.52
$\text{BeF}_2\text{—FH}$	2.188	-14.126	10.347	-0.002	0.023	-2.298	0.203	1.54
$\text{BeF}_2\text{—ClH}$	2.195	-14.136	11.192	0.005	0.013	-1.452	0.479	—
$\text{BeF}_2\text{—BrH}$	2.195	-14.134	11.311	0.005	0.016	-1.333	0.349	—
$\text{BeCl}_2\text{—NH}_3$	2.244	-14.130	11.937	0.002	0.019	-3.203	0.778	2.23
$\text{BeCl}_2\text{—OH}_2$	2.235	-14.118	11.793	-0.007	0.031	-3.348	0.681	2.24
$\text{BeCl}_2\text{—PH}_3$	2.257	-14.131	12.991	0.015	0.018	-2.150	0.703	2.12
$\text{BeCl}_2\text{—SH}_2$	2.250	-14.124	12.814	0.007	0.025	-2.327	0.662	2.11
$\text{BeCl}_2\text{—FH}$	2.228	-14.106	12.351	-0.014	0.043	-2.790	0.532	2.17
$\text{BeCl}_2\text{—ClH}$	2.240	-14.118	13.002	-0.003	0.031	-2.138	0.549	2.06
$\text{BeCl}_2\text{—BrH}$	2.242	-14.120	13.361	0.000	0.029	-1.779	0.543	2.02

## Mutual penetration of beryllium and acceptor atoms

To estimate the penetration of beryllium and the acceptor atoms (denoted by Y which refers to N, O, S, P, F, Cl or Br in  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{H}_2\text{S}$ ,  $\text{PH}_3$ ,  $\text{HF}$  or  $\text{HBr}$ , respectively) the non-bonding radii ( $r_{\text{Be}}^0$  and  $r_{\text{Y}}^0$ ) have been compared to the corresponding bonding radii ( $r_{\text{Be}}$  and  $r_{\text{Y}}$ ). The non-bonding radius of an atom is defined as the distance from its nucleus to a 0.001 a.u. contour in the isolated molecule. For beryllium, this radius evaluated in the direction perpendicular to the  $\text{BeX}_2$  molecular axis, i.e., in the direction which Be bond is formed. The bonding radii are taken as the distance from a nucleus to the BCP in question. Now, the penetrations of Be and Y (denoted by  $\Delta r_{\text{Be}}$  and  $\Delta r_{\text{Y}}$ ) are defined as  $\Delta r_{\text{Be}} = r_{\text{Be}}^0 - r_{\text{Be}}$  and  $\Delta r_{\text{Y}} = r_{\text{Y}}^0 - r_{\text{Y}}$ , respectively. The values of  $\Delta r_{\text{Be}}$  for the studied complexes, has been listed in Table 2. The positive sign of these values (and those of  $\Delta r_{\text{Y}}$ ) reveal that the beryllium and Y atoms penetrate each other when a beryllium bond is formed. In addition, the  $\Delta r_{\text{Be}}$  values are considerably higher than the reported values of  $\Delta r_{\text{H}}$  for hydrogen bonded complexes [29].

## Charge of beryllium atom

As stated earlier, when a hydrogen bond is formed, the hydrogen atom loses electrons, or in better words, its electronic population,  $N(H)$ , decreases. The changes in the electronic population of beryllium,  $\Delta N(\text{Be})$ , are given in Table 2.

Unlike the hydrogen atom in the hydrogen bonds, the electronic population of beryllium, in most cases, increase (that is  $\Delta N(Be)$  become positive) upon formation of beryllium bonds. The only exception is the complex between  $Cl_2Be$  and  $H_2O$  in which  $\Delta N(Be)$  is negative. It should be mentioned that other negative and zero values of  $\Delta N(Be)$  in Table 2 correspond to the complexes of  $X_2Be$  with hydrogen halides, in which there is no BCP between beryllium atom and the base (and according to the first criterion cannot be regarded as beryllium bonds) or the beryllium bond affected by a secondary interaction (halogen bond in  $F_2Be...FH$  and  $F_2Be...ClH$  and hydrogen bond in  $Cl_2Be...ClH$ ).

#### Energy of beryllium atom

The negative values of  $\Delta E(Be)$  (difference between atomic energy of beryllium in the complex and isolated  $BeX_2$ ) in Table 2 show that the beryllium atom, similar to hydrogen in hydrogen bonds, is destabilized upon complex formation.

#### Dipolar polarization of beryllium atom

The atomic dipole moment in  $BeX_2$  monomers is zero and as indicated in Table 2, the value of dipolar polarization (magnitude of atomic dipole moment) of beryllium increases upon formation of a complex.

#### The volume of beryllium atom

The final criterion of hydrogen bonds states that the volume of hydrogen atom decreases upon formation of hydrogen bonds. For the beryllium bonded complexes, the changes in the volume of beryllium atom,  $\Delta V(Be)$ , has been collected in Table 2. As can be seen, like for hydrogen, the volume of beryllium decreases when a beryllium bond is formed.

### Conclusions

In the current work, the nature of beryllium bonds formed between  $BeX_2$  ( $X$  is H, F and Cl) and some Lewis bases ( $NH_3$ ,  $H_2O$ ,  $H_2S$ ,  $PH_3$ , HF, HCl and HBr) have been investigated. The distribution of the Laplacian of electron density of  $BeX_2$  monomers shows that there is a region of charge depletion (hole) around the Be atom, which, according to Laplacian complementary principal, can interact with a region of charge concentration (lump) of an atom (N, O, S, P and sometimes halogens) in another molecule ( $NH_3$ ,  $H_2O$ ,  $H_2S$ ,  $PH_3$  or hydrogen halides) and consequently, form a beryllium bond. The molecular graphs of the investigated complexes indicate that beryllium in  $BeH_2$  and  $BeF_2$  can form a “beryllium bonds” with O, N and P atoms but not with halogens. In addition, eight criteria based on QTAIM

properties, including the values of electron density and its Laplacian at the BCP, penetration of beryllium and acceptor atom, charge, energy, volume and first atomic moment of beryllium atom, have been considered and compared with the corresponding ones in conventional hydrogen bonds. These bonds share many common features with very strong hydrogen bonds, however some differences are also observed. It has also been shown that the beryllium bonds are partially electrostatic and partially covalent.

### References

- Buckingham AD, Fowler PW, Hutson JM (1988) Chem Rev 88:963–988
- Philp D, Stoddart JF (1996) Angew Chem Int Ed Engl 35:1155–1196
- Rudkevich DM (2004) Angew Chem Int Ed Engl 43:558–571
- Saalfrank RW, Maid H, Scheurer A (2008) Angew Chem Int Ed Engl 47:8794–8824
- Llanes-Pallas A, Piot CA, Balbakra A, Listorti A, Prato M, Samori P, Armaroli N, Bonifazi DJ (2009) J Am Chem Soc 131:509–520
- Jeffrey GA (1997) An Introduction to Hydrogen Bonding. Oxford University Press, New York
- Desiraju GR, Scheiner T (1999) The Weak Hydrogen Bond in Structural Chemistry and Biology. Oxford University Press, Oxford
- Alkorta I, Rozas I, Elguero J (1998) Chem Soc Rev 27:163–170
- Grabowski SJ (2006) Hydrogen bonding -new insights vol 3. Springer, Berlin
- Neumuller B, Weller F, Dehnicke KZ (2008) Anorg Allg Chem 634:662–668
- Holleman F, Wiberg N, Wiber E (2001) Inorganic chemistry. Academic, Cambridge
- Housecroft C, Sharpe AG (2008) Inorganic Chemistry, 3rd edn. Prentice-Hall, New York
- Grabowski SJ (2000) J Mol Struct 553:151–156
- Dressel MP, Nogai S, Berger RJF, Schmidbaur HZ (2003) Naturforsch (B) 58:173–182
- Yáñez M, Sanz P, Mo O, Alkorta I, Elguero J (2009) J Chem Theor Comput 5:2763–2771
- Bader RFW (1990) Atoms in molecules; a quantum theory. Clarendone, Oxford
- Becke AD, Edgecombe KE (1990) J Chem Phys 92:5397–5403
- Silvi B, Savin A (1994) Nature 371:683–686
- Reed AE, Curtis LA, Weinhold F (1988) Chem Rev 88:899–926
- Koch U, Popelier PLA (1995) J Phys Chem 99:9747–9754
- Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Montgomery JA Jr, Vreven T, Kudin KN, Burant JC, Millam JM, Iyengar SS, Tomasi J, Barone V, Mennucci B, Cossi M, Scalmani G, Rega N, Petersson GA, Nakatsuji H, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Klene M, Li X, Knox JE, Hratchian HP, Cross JB, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann RE, Yazyev O, Austin AJ, Cammi R, Pomelli C, Ochterski JW, Ayala PY, Morokuma K, Voth GA, Salvador P, Dannenberg JJ, Zakrzewski VG, Dapprich S, Daniels AD, Strain MC, Farkas O, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Ortiz JV, Cui G, Baboul AG, Clifford S, Cioslowski J, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen

- W, Wong MW, Gonzalez C, Pople JA (2004) Gaussian 03, Revision B.03. Gaussian Inc, Wallingford
22. Keith TA (2011) AIMAll (standard mode), 11.02.27, [aim.tkgristmill.com](http://aim.tkgristmill.com)
23. Biegler-König F, Schönbohm J (2002) AIM2000 Program Package, Ver. 2.0. [www.aim2000.de](http://www.aim2000.de)
24. Graña MA, Mosquera RA (1999) J Chem Phys 110:6606–6616
25. Vila A, Mosquera RA (2001) J Chem Phys 115:1264–1273
26. Bader RFW, Cheng C (1989) J Phys Chem 93:2946–2956
27. Carroll MT, Cheeseman JR, Osman R, Wienstein H (1989) J Phys Chem 93:5120–5123
28. Eskandari K, Zariny H (2010) Chem Phys Lett 492:9–13
29. Popelier P (2000) Atoms in molecules, an introduction. Prentice-Hall, Harlow
30. Popelier PLA (1998) J Phys Chem 102:1873–1878
31. Popelier PLA, Logothetis G (1998) J Organomet Chem 555:101–111
32. Pakiari AH, Eskandari K (2006) J Mol Struct (THEOCHEM) 759:51–60