Ab Initio Study of Lithium-Bonded Complexes with Carbene as an Electron Donor

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The complexes H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) have been studied with quantum chemical calculations at the MP2/6-311++G(d,p) level. A new type of lithium bond was proposed, in which the carbene acts as the electron donor. This new type of lithium bond was characterized in view of the geometrical, spectral and energetic parameters. The Li−X bond elongates in all lithium bonded complexes. The Li−X stretch vibration has a red shift in the complexes H_2C-LiX (X = H, OH, F); however, it exhibits a blue shift in the complexes H_2C-LiX (X = Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2). The binding energies are in a range of 16.88−21.13 kcal/mol, indicating that the carbene is a good electron donor in the interaction. The energy decomposition analyses show that the electrostatic contribution is largest, polarization counterpart is followed, and charge transfer is smallest. The effect of substitution and hybridization on this type of lithium bond has also been investigated.

1. Introduction

Intermolecular interactions are of great important in biological and chemical systems;[1] thus in recent years much attention has been focused on them with methods of experiment and theory. Although the geometry and strength of interaction are the main topic of interest, the nature and origin of such interactions have been focused recently[2−4] due to presence of advanced theoretical procedures. Hydrogen bonds are not an exception to this although they are abundant and well studied.

Lithium bonding suggested in 1959 by Shigorin[5] is an interaction analogous to hydrogen bonding in view of the fact that lithium is a congener of hydrogen. Its existence was theoretically predicted in 1970 by Kollman et al.[6] and experimentally confirmed in 1975 by Ault and Pimentel.[7] Kollman et al.[6] thought that LiF could bond to a suitable base using Hartree−Fock calculations. In complexes XLi-Y (X = Cl and Br, Y = H_2O, H_3N, $(CH_3)_2O$, $(CH_3)_3N$), a large red shift of the Li−X stretching frequency was observed in matrix isolation infrared spectra by Ault and Pimentel.[7] Although the concept of lithium-bond has been accepted and is important in many fields, study of the lithium-bond interaction is relatively rare with comparison to that of the hydrogen bond.

Like the hydrogen bond, the lithium bond is also classified into conventional and unconventional. The study of the conventional lithium bond, where a lone pair on an electronegative atom acts as an electron donor, is the earliest and most studied in lithium-bonded systems.[8−10] The π lithium bond formed between lithium and π electron provided by acetylene, ethylene, benzene, furan, or thiophene also obtained much attention.[11−13] A new kind of single-electron lithium bonding in H_3C-LiY (*Y* = H, F, OH, CN, NC, and CCH) complexes was predicted and characterized by Li et al.[14] Very recently, we proposed another new kind of lithium bonding, in which HMgH molecule acts as an electron donor, by employing quantum chemical calculations.[15]

Carbene is a highly reactive organic molecule containing a carbon atom with six valence electrons, in which methylene is the simplest one. Although carbenes are species with short lifetimes, some stable carbenes were detected at room temperature.[16] In general, there are two types of carbenes: singlet or triplet carbenes. Hydrogen bond with singlet carbene as an electron donor has been confirmed due to presence of a free electron pair in the singlet carbene.[17] It is shown that carbene is a good electron donor in formation of hydrogen bond. However, to the best of our knowledge, the study of the lithium bond with carbene as an electron donor is rare.

In view of the close parallelism of lithium bond with hydrogen bond, it is reasonable to deduce that the lithium bond with carbene as an electron donor also exists. For confirmation of this, we employ quantum chemical calculations to study the complex of H_2C-LiX, where X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2. Although carbene has two classes: singlet and triplet, we only consider the singlet carbene due to presence of a free electron pair in singlet carbene. We also perform an analysis with the quantum theory of atoms in molecules (QTAIM) for these complexes to further confirm the existence of lithium bond. Finally, we perform energy decomposition analysis to trace the nature of such lithium bonding. We think that this study can enrich the knowledge on lithium bonding interactions.

2. Theoretical Methods

All calculations were performed with the aid of Gaussian 03 suite of program.[18] The complexes of H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) have been optimized at the MP2/6-311++G(d,p) level. This method has been employed to study the structures and properties of a variety of lithium bonds.[10,13,15] Then the corresponding frequency calculations were carried out at the same level to ensure that the complex structures are true minima. The interaction energies

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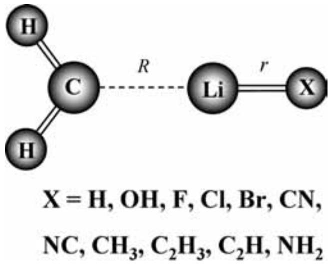

Figure 1. Optimized structures of the H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) complexes.

TABLE 1: Binding Distance (*R*, Å), Li—X Bond Length (*r*, Å), Li—X Stretch Frequency (*v*, cm^{-1}), and Infrared Intensity (*I*, km/mol) in the Eleven Complexes Calculated at the MP2/6-311++G(d,p) Level

	R	r^a	v^a	I^a
H_2C-LiH	2.2172	1.6254(0.0260)	1365(−67)	350(128)
H_2C-LiOH	2.2182	1.6305(0.0241)	915(−8)	192(17)
H_2C-LiF	2.2164	1.6238(0.0248)	876(−3)	167(11)
H_2C-LiCl	2.1869	2.0494(0.0273, 0.0278)[b]	711(51, 37)	139(−1)
H_2C-LiBr	2.1857	2.2181(0.0299, 0.0308)	648(79, 66)	118(−2)
H_2C-LiCN	2.1953	1.9605(0.0282, 0.0305)	672(54, 41)[b]	128(1)
H_2C-LiNC	2.1968	1.8238(0.0272, 0.0293)	725(38, 28)	170(−3)
H_2C-$LiCH_3$	2.2182	2.0139(0.0240, 0.0252)	665(40, 31)	56(24)
H_2C-$LiHCCH_2$	2.2096	1.9919(0.0229, 0.0245)	684(43, 33)	79(17)
H_2C-LiCCH	2.2053	1.9383(0.0282, 0.0307)	689(43, 30)	136(6)
H_2C-$LiNH_2$	2.1995	1.7841(0.0253, 0.0267)	810(9, 2)	95(123)

[a] Data in parentheses are the difference between the complex and the monomer. [b] Data of the second column in parentheses are obtained from by the CP-corrected geometry and frequency calculations.

were calculated to be the difference between the energy of the complex and the energy sum of the respective monomers. The interaction energies were corrected for the basis set superposition error (BSSE) following the counterpoise procedure proposed by Boys and Bernardi.[19] Topological parameters, including electron densities and their Laplacians, were calculated with the AIM 2000 software.[20] Energy decomposition analysis has also been carried out with Gamess program[21] to explore the bonding nature of the H_2C-LiX complex.

3. Results and Discussion

3.1. Bond Lengths and Infrared Spectra. Figure 1 shows the sketch map of the H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) complexes. Two structure parameters (binding distance *R* and Li—X bond length *r*) are marked in the figure. Their data and their changes due to the complexation are given in Table 1. The binding distance is in a range of 2.1857−2.2182 Å, which is much smaller than the sum of the van der Waals radii of the C and Li atoms (about 3.5 Å). This means that there is a strong attractive force between the two subunits, which is responsible for the stability of the complexes. We named it a carbene lithium bond based on the fact that the carbene acts as an electron donor and the Li atom is the lithium donor in the interaction. The binding distance is calculated to be 2.2172 Å in the H_2C-LiH complex. The presence of the electron-donating group (OH) in the LiX molecule makes a 0.0010 Å increase of the binding distance, whereas the electron-withdrawing groups (F, CN, and NC) result in a shortening of the binding distance. The binding distance increases in H_2C-$LiCH_3$ complex, whereas it decreases in H_2C-$LiHCCH_2$ and H_2C-LiCCH complexes. For the three H_2C-LiR complexes, the binding distance in H_2C-LiCCH complex is smallest; that in H_2C-$LiHCCH_2$ complex is followed; that in H_2C-$LiCH_3$ complex is largest. An interesting feature of these results is the shortening binding distance as the X (X = F, Cl, and Br) atoms become larger, which corresponds to a decreasing value of the halogen atom electronegativity.

As expected, the Li—X bonds are lengthened in all complexes. The elongation of the Li—X bond varies from 0.0229 to 0.0299 Å. This elongation is larger than that in the lithium-hydride lithium bond[15] and single-electron lithium bond.[14] The Li—H bond elongation is 0.0260 Å in H_2C-LiH complex. The electron-donating groups (OH and NH_2) result in a decrease of the Li—X bond elongation. The F electron-withdrawing group makes it decrease, whereas the CN and NC electron-withdrawing groups cause it increase. The Li—C bond elongation in H_2C-LiCCH complex is larger than that in H_2C-$LiCH_3$ and H_2C-$LiHCCH_2$ complexes. The Li—X bond elongation in the three halogen-containing complexes increases in the following order: H_2C-LiF < H_2C-LiCl < H_2C-LiBr. According to the above analyses, it is seen that the Li—X bond elongation is not completely consistent with the change of the binding distance.

Table 1 also shows the Li—X stretch frequency and its infrared intensity in the H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) complexes. The Li—X stretch frequency is real and not scaled. Accompanied with the Li—X bond elongation in the complex formation, the Li—X stretch vibration (X = H, OH, F) moves to low frequency, whereas the Li—X stretch vibration (X = Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) shifts to high frequency. A similar result is also found in H_3C-LiY (Y = H, F, OH, CN, NC, and CCH) complexes[14] and HMgH···LiX (X = H, OH, F, CCH, CN, and NC) complexes.[15] It is an abnormal blue shift of the Li—X stretch frequency (X = Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2), which is not consistent with the Li—X bond elongation. This inconsistency was also observed in some other lithium-bonded complexes.[22,23] Guo and coauthors[22] thought the possible reason for this inconsistency is the coupling between the Li—X vibration and vibration of other bonds. Such explanation may be not right to be used here because the Li—C stretch frequency is much lower than that of other bonds, such as C≡N. In ref 14, the authors tested the reliability of the abnormal blue shift with five different methods including QCISD/aug-cc-pVDZ. At all cases, the abnormal blue shift occurs. The results obtained from the CP-corrected gradient optimization are thought to be more reliable than those from the standard optimization.[4] Thus we also considered the effect of the CP-corrected gradient optimization on the inconsistency. The results (Table 1) show that this inconsistency is still present with this method, and the difference between the two methods is that the Li—X bond elongation is larger and the blue shift of the Li—X stretch frequency is smaller with the CP method. We think that the origin of such elongated but blueshifted lithium bond still needs to be explored in the future.

The red shift of the Li—X stretch frequency is 67 cm^{-1} in the H_2C-LiH complex, which is larger than that in the H_3C-LiH (26.5 cm^{-1})[14] and HMgH-LiH complexes (56 cm^{-1}).[15] Whether in the H_2C-LiF complex or in the H_2C-LiOH complex, this red shift decreases greatly. This effect is different from that in hydrogen bond. The blue shift of the Li—X stretch frequency is largest in the H_2C-LiBr complex. The blue shift in the H_2C-$LiHCCH_2$ complex amounts to that in the H_2C-LiCCH complex, both being larger than that in the H_2C-$LiCH_3$ complex. These blue shifts are larger than those found in the corresponding single-electron lithium bond[14] and lithium−hydrogen lithium bond.[15]

TABLE 2: Interaction Energies (Δ*E*, kcal/mol) and Dipole Moments (*μ*, D) of the Lithium Bonds in the 11 Complexes Calculated at the MP2/6-311++G(d,p) Level

	μ	ΔE_{MP2}	BSSE	ΔE_{corr}	ΔE_{HF}
H_2C-LiH	9.11	−20.17	2.19	−17.98	−19.91
H_2C-LiOH	7.71	−19.38	2.50	−16.88	−18.43
H_2C-LiF	9.66	−20.59	2.63	−17.97	−20.04
H_2C-LiCl	10.60	−22.91	2.87	−20.04	−22.48
H_2C-LiBr	10.94	−23.28	2.61	−20.67	−22.88
H_2C-LiCN	12.96	−23.42	2.41	−21.01	−23.42
H_2C-LiNC	12.16	−23.48	2.35	−21.13	−22.54
H_2C-$LiCH_3$	9.17	−19.76	2.36	−17.40	−19.09
H_2C-$LiHCCH_2$	9.40	−20.73	2.40	−18.32	−20.08
H_2C-LiCCH	9.61	−21.56	2.46	−19.10	−21.13
H_2C-$LiNH_2$	8.06	−20.00	2.43	−17.57	−18.81

Upon the complex formation, the infrared intensity increases whether the Li−X stretch vibration exhibits a red shift or a blue shift. The intensity increase is largest in the H_2C-LiH complex and smallest in the H_2C-LiCN complex. However, the infrared intensity decreases a little in the three complexes (H_2C-LiCl, H_2C-LiBr, and H_2C-LiNC). No systemic changes are present for the intensity increase.

3.2. Interaction Energy. The interaction energy is one of the most important measurements for characterizing the intermolecular interaction. Table 2 presents the interaction energies in the H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) complexes. The interaction energies at the MP2 theory were corrected for the BSSE. The uncorrected interaction energies are in a range of 19.38−23.48 kcal/mol and the BSSE amounts to less than 13% of the raw interaction energy. This portion is smaller than that in hydrogen bond for the reason that the lithium bond is much stronger.

The corrected interaction energy in the H_2C-LiH complex is calculated to be −17.98 kcal/mol. It is larger than that in the HMgH-LiH (−13.07 kcal/mol)[15] and H_3C-LiH complexes (−5.72 kcal/mol).[14] The interaction energy in the H_2C-LiF complex almost equals that in the H_2C-LiH complex, and it is larger than that in the C_2H_4−LiF complex (−10.5 kcal/mol).[12] This indicates that the carbene is as good of an electron donor as that in hydrogen[17] and halogen bonds.[24] As the H atom in LiH molecule is replaced by an electron-donating group such as OH and NH_2, the interaction energy decreases. As the H atom in LiH molecule is substituted by an electron-withdrawing group such as CN and NC, the interaction energy increases. This substitution effect is similar to that in hydrogen bond[25] and other types of lithium bonds.[14,15]

The methyl group plays an interesting role in the formation of OH$\cdots$O hydrogen bond in methanol-methyl sulfoxide complex: the methyl group in the electron donor is electron-donating, whereas that in the proton donor is electron-withdrawing, both making a positive contribution.[26] In the CH_3NH_2-LiF complex,[27] the methyl group also plays a positive role in the formation of lithium bond. As the H atom in LiH molecule is replaced by a methyl group, the interaction energy is decreased to be −17.40 kcal/mol. This shows that the methyl group in the lithium donor plays a negative contribution in formation of carbene lithium bond, which is different from that in the OH$\cdots$O hydrogen bond. The natural population charge of methyl group is −0.884 and −0.857 e in $LiCH_3$ and H_2C-$LiCH_3$, respectively. Clearly, the methyl group negative charge decreases upon complexation. This means that the methyl group in the lithium donor is electron-donating, thus making a negative contribution.

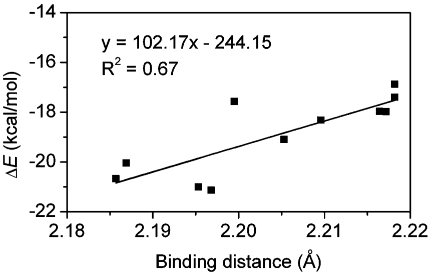

Figure 2. Relationship between the interaction energy and the binding distance.

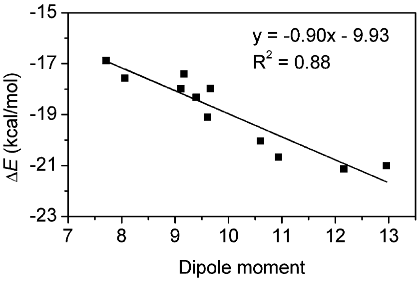

Figure 3. Relationship between the interaction energy and the dipole moment.

The properties of XH$\cdots$Y hydrogen bonds not only depend on the properties of X, Y, and H but are related with substitution and hybridization.[28] For CH$\cdots$O, CH$\cdots$N, CH$\cdots$F, and CH$\cdots$S hydrogen bonds,[29−31] hydrogen bonding strength increases in the following sequence: C(sp^3)-H < C(sp^2)-H < C(sp)-H. The interaction energy in the H_2C-$LiCH_3$, H_2C-$LiHCCH_2$, and H_2C-LiCCH complexes is −19.09, −20.08, and −21.13 kcal/mol, respectively. Evidently, the strength of the lithium bond also conforms to the above sequence.

In hydrogen bonds, the interaction energy has a linear relationship with the binding distance. Similarly, a linear relationship is also observed between them in this type of lithium bond (Figure 2) as that in the lithium−hydrogen lithium bond.[15] This shows a similarity between lithium bond and hydrogen bond.

The dipole moments of the complexes are also given in Table 2. Figure 3 shows the relationship between the binding energy and the dipole moment. An approximate linear relationship is found, indicating that the electrostatic and polarization interactions are responsible for the stability of the complexes. To further approve this, the interaction energies in these complexes are also calculated at the Hartree−Fock level. These data are also presented in Table 2. The values of the ΔE_{HF} are more than 94% of the ΔE_{MP2}, indicating a main contribution of electrostatic energy to the interaction energy.

3.3. QTAIM Analyses. The topological characterization of conventional lithium bonding has been studied in several LiF complexes.[10] The result shows that the electron density at lithium bond critical points (BCPs) is about half of its value in the hydrogen bonding analogues, suggesting a dominant role of electrostatic interaction rather than charge transfer in the lithium-bonded complexes. On the basis of the fact that there is a BCP between the donor lithium atom and the C atom in the H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH_3, C_2H_3, C_2H, NH_2) complex, a topological analysis of the electron density further validates the existence of lithium bonds in all of the complexes. The properties at the C$\cdots$Li and Li−X BCPs have been analyzed in terms of the following two parameters: the electron density (ρ) and its Laplacian ($\nabla^2\rho$). The results are collected in Table 3.

The values of the ρ(C$\cdots$Li) are calculated to be in a range of 0.0221−0.0244 au, whereas the values of the $\nabla^2\rho$(C$\cdots$Li)

TABLE 3: Electron Densities (ρ, au) and Their Laplacians ($\nabla^2\rho$, au) at the Bond Critical Points in the H_2C-LiX Complexes Calculated at the MP2/6-311++G(d,p) Level

	ρ(C···Li)	$\nabla^2\rho$(C···Li)	ρ(Li−X)	$\nabla^2\rho$(Li−X)
H_2C-LiH	0.0223	0.1198	0.0373(0.0395)	0.1501(0.1656)
H_2C-LiOH	0.0221	0.1199	0.0599(0.0642)	0.5871(0.6415)
H_2C-LiF	0.0224	0.1200	0.0623(0.0656)	0.5995(0.6596)
H_2C-LiCl	0.0243	0.1303	0.0423(0.0449)	0.2519(0.2745)
H_2C-LiBr	0.0244	0.1310	0.0353(0.0376)	0.1832(0.2000)
H_2C-LiCN	0.0241	0.1276	0.0404(0.0430)	0.2190(0.2383)
H_2C-LiNC	0.0239	0.1273	0.0452(0.0484)	0.3284(0.3600)
H_2C-LiCH$_3$	0.0223	0.1195	0.0415(0.0434)	0.1978(0.2314)
H_2C-LiHCCH$_2$	0.0229	0.1220	0.0426(0.0448)	0.2139(0.2303)
H_2C-LiCCH	0.0233	0.1238	0.0434(0.0461)	0.2341(0.2551)
H_2C-LiNH$_2$	0.0232	0.1256	0.0525(0.0559)	0.3824(0.4161)

are all positive and vary from 0.1195 au to 0.1310 au. These values are within the common accepted values for hydrogen bonds,[32] thus showing the typical closed-shell interactions in these complexes. The linear correlations between the interaction energy and the topological parameters at the corresponding BCP have been established for H-bond interactions.[33] A linear relationship is also found between the electron densities at the C···Li BCPs and the corresponding interaction energies of the complexes (Figure 4). The value of the square correlation coefficient is 0.82. That is to say, the electron density at the C···Li BCP is also a good indication of the strength of lithium bonding interactions.

For all complexes, the values of the ρ(Li−X) range in 0.0353−0.0623 au, whereas the values of the $\nabla^2\rho$(Li−X) vary from 0.1501 to 0.5995 au. These values at the Li−X BCPs are much larger than those at the C···Li BCPs. They decrease relative to those in the respective monomer. The result is an indication of the Li−X bond weakening, which supports the elongation of the Li−X bond upon complexation.

3.4. Energy Decomposition Analyses. To further understand the nature of this type of lithium bonding, the interaction energies in these complexes have been studied with the Morokuma scheme.[21] This method can partition molecular interaction energies into electrostatic energy (ES), exchange repulsion energy (EX), polarization energy (PL), charge transfer energy (CT), and high-order coupling energy (MIX). The ES term represents the Coulombic interaction between the charge distribution of the two subunits, and the EX approximately corresponds to the steric repulsion between the two charge clouds. The PL corresponds to the internal redistribution of the charge clouds of the complex components; the CT is connected with the charge density shifts from one molecule to the other, and the MIX term represents the higher-order repulsive interactions. The results are summarized in Table 4. The total interaction energies obtained with this method are consistent with those by the supermolecular method.

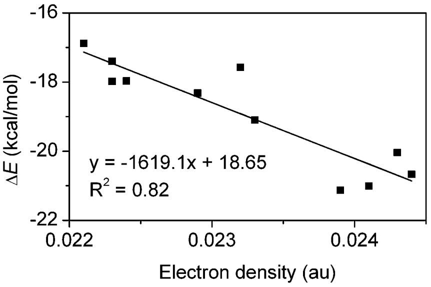

Figure 4. Relationship between the interaction energy and the electron density at the C···Li BCP.

TABLE 4: ES, EX, PL, CT, MIX, and ΔE in the 11 Complexes (All Terms Are in kcal/mol)

	ES	EX	PL	CT	MIX	ΔE
H_2C-LiH	−25.22	11.41	−14.31	−1.11	9.70	−19.53
H_2C-LiOH	−24.00	11.05	−10.27	−1.54	6.63	−18.14
H_2C-LiF	−25.32	11.34	−11.21	−1.35	6.97	−19.57
H_2C-LiCl	−27.55	12.45	−13.61	−1.56	8.93	−21.54
H_2C-LiBr	−28.05	12.56	−14.28	−1.57	9.15	−22.19
H_2C-LiCN	−28.18	12.12	−14.18	−2.60	9.96	−22.87
H_2C-LiNC	−27.63	12.41	−13.52	−2.32	9.32	−21.74
H_2C-LiCH$_3$	−24.53	11.30	−19.36	−1.48	15.44	−18.63
H_2C-LiHCCH$_2$	−25.35	11.40	−15.33	−1.98	11.61	−19.64
H_2C-LiCCH	−26.24	11.58	−12.45	−2.91	9.16	−20.86
H_2C-LiNH$_2$	−24.69	11.61	−12.02	−1.77	8.89	−17.98

As can be seen in Table 4, the components of the ES, PL, and CT are negative, whereas those of the EX and MIX are positive. This indicates that the ES, PL, and CT play a positive contribution to the binding, whereas the EX and MIX are a negative contribution. The ES contribution is largest; the PL contribution is followed, and the CT contribution is smallest. This shows that the nature of this type of lithium bond is mainly electrostatic. Additionally, the polarization also plays an important contribution.

For each complex, the electrostatic energy term outweighs the exchange term, and the higher-order repulsion terms are very important. The ES is largest in the H_2C-LiCN complex and smallest in the H_2C-LiOH complex. The CT is more negative for the Li donor adjoined with a π electron than that for the other Li donor. The PL term is largest in the H_2C-LiCH$_3$ complex and smallest in the H_2C-LiOH complex. As the C hybridization varies from sp^3 through sp^2 to sp, the ES and CT are more negative, the PL is less negative, the EX is more positive, and the MIX is less positive.

4. Conclusions

A new type of lithium bond has been predicted and characterized in H_2C-LiX (X = H, OH, F, Cl, Br, CN, NC, CH$_3$, C$_2$H$_3$, C$_2$H, NH$_2$) complexes at the MP2/6-311++G(d,p) level. This new type of lithium bond is named as a carbene lithium bond. Upon the complex formation, the Li−X bond is lengthened. Accompanied with the elongation, the H_2C-LiX (X = H, F, OH) complex exhibits a red shift of the Li−X stretching frequency, whereas a blue shift of the Li−X stretching frequency is observed in the H_2C-LiX (X = Cl, Br, CN, NC, CH$_3$, C$_2$H$_3$, C$_2$H, NH$_2$) complex. The binding energies of carbene lithium bonds, depending on the chemical environment of the lithium, range from 16.88 to 21.01 kcal/mol. QTAIM analyses have also been carried out for each complex. A correlation of the binding energy with the electron density at the C···Li BCP has been established, which may provide some insights into the nature of the interaction. The nature of this type of lithium bond is further unveiled with the energy decomposition analyses. Although the polarization interaction has a great contribution to the formation of the interaction, the nature of the interaction is electrostatic. By consideration that the carbene is an intermediate in chemical reactions and methyllithium is a catalyst, thus the study of the interaction between the carbene and methyllithium is helpful to understand the mechanism in some chemical reactions. We believe that this study enriches the knowledge on lithium bond interactions and need some support from future experimental work.

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