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Research Article

Theoretical Prediction for Synthetic Realization: Pyramidal Systems ClE[E'_4R_4] (E = B–Ga, E' = C–Ge, R = $SiMe_3$, $SiMe^tBu_2$): A DFT Study

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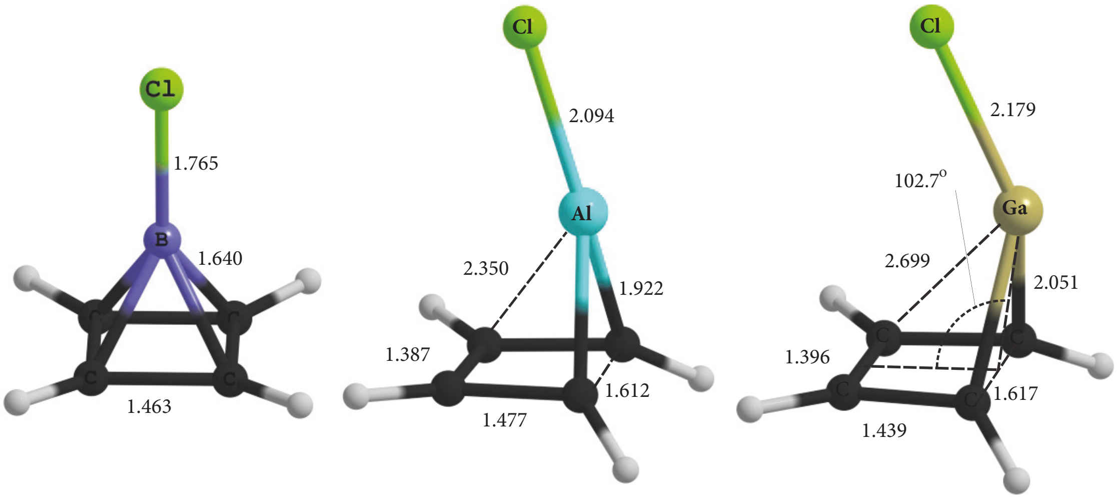
Structure and bonding of hybrid group 13/14 pyramidal molecules ClE[E'_4R_4] (E = B–Ga, E' = C–Ge, R = $SiMe_3$, $SiMe^tBu_2$) were studied by DFT calculations. Six pyramidal structures are suggested for their potential synthetic realization.

1. Introduction

Among the great variety of polyhedral cluster compounds, pyramidanes are of particular importance due to their unusual structures and bonding situations, especially nonclassical interaction mode between their apexes and bases [1–4]. However, despite such evident interest, pyramidanes eluded their synthetic realization until very recently and became synthetically accessible only several years ago [5–13]. The closest approximation to the most challenging but still hypothetical all-carbon pyramidanes C[C_4R_4] represents derivatives in which apical carbon is replaced with the main group element. To date, neutral pyramidanes of the type E[$C_4(SiMe_3)_4$] (E = Ge, Sn, Pb) [5, 14] were synthesized and fully structurally characterized. Moreover, pyramidanes in which the basal carbon atoms are replaced with the heavier group 14 elements (Si, Ge, and Sn) were also approached both experimentally and theoretically [14, 15]. Since the first investigations on the pyramidanes, it quickly became apparent that the structural and chemical peculiarities of the latter are totally dictated by the particular nature of their apical and basal atoms, whereas stability of pyramidanes is governed by the substituents at the basal atoms. Thus, for example, for the model E[E'_4H_4] (E = C–Pb, E' = C, Si, Ge) pyramidanes, square-pyramidal C_{4v} energy minima structures were found only for pyramidanes with the carbon base (E' = C; E = C–Pb), whereas with the heavier atoms at the base (E' = Si, Ge; E = C–Pb) the optimized molecule represents a distorted structure [14]. However, substituents at the basal atoms play a decisive role in the overall stabilization of the square-pyramidal structures, which actually takes place upon the successive increase in the size of substituents on going from H to H_3Si to Me_3Si to $^tBu_2MeSi$. Thus, for example, most pyramidal structures E[$Si_4(SiMe_2{}^tBu)_4$] (E = Si–Sn) correspond to the energy minima on the potential energy surface (PES), whereas for the structures E[$Ge_4(SiMe_2{}^tBu)_4$] stationary points can be found as either energy minima or transition states (TS) with low inversion barriers [14]. Further extending the range of pyramidal structures family, we also synthesized cationic pyramidanes of the type $\{E[C_4(SiMe_3)_4]\}^+\bullet[A]^-$ (E = P, Sb; $[A]^-$ = $[B(C_6F_5)_4]^-$, $[Sb_2F_7]^-$)[16, 17] Moreover, very recently the first (chloro)borapyramidane ClB[$C_4(SiMe_3)_4$] was also reported [18], being the first and still remaining the single representative of the neutral pyramidanes with the group 13 elements at the top of the square pyramid. Given very promising structural and chemical properties of the borapyramidane, it would be very challenging to expand the scope of the reaction and prepare a whole series of the hybrid group 13/14 elements pyramidanes (group 13 elements at the apex and group 14 elements at the base) and study the general

Table 1: Numbers of imaginary frequencies (NI) and relative energies towards closest minima (ΔE, kcal mol^{-1}) for model pyramidal systems **1–9** (C_{4v} symmetry).

Structure	E = B	E = Al	E = Ga
$ClE[C_4H_4]$	**1**, NI = 0	**2**, NI = 2, ΔE = 0.8	**3**, NI = 2, ΔE = 13.0
$ClE[Si_4H_4]$	**4**, NI = 3, ΔE = 2.2	**5**, NI = 3, ΔE = 11.1	**6**, NI = 3, ΔE = 10.5
$ClE[Ge_4H_4]$	**7**, NI = 3, ΔE = 12.9	**8**, NI = 3, ΔE = 26.5	**9**, NI = 3, ΔE = 41.3



1, C_{4v} **2**, C_s **3**, C_s

Figure 1: Optimized geometries (bond lengths are in Å) of minima structures **1–3**.

trends within this series. However, it seems reasonable before pursuing experimental attempts to study the accessibility of such hybrid pyramidanes from a computational viewpoint. But such highly desirable theoretical treatment is still lacking; therefore we decided to undertake a systematic study of the general trends in stability, structural, and bonding features of hybrid pyramidanes depending on the nature of the apical and basal atoms and substituents. In this work, we report on the systematic DFT study of structure, stability, and bonding features of the series of hybrid neutral pyramidanes $ClE[E'_4R_4]$ (E = B–Ga; E' = C–Ge; R = H, $SiMe_3$, $SiMe^tBu_2$) possessing C_4-symmetry.

2. Computational Details

All computations were performed with the Gaussian 16 [19] suite of programs at the B3LYP/Def2TZVP level [20–24]. Our previous works [14–18] showed that this level of theory is well-suited to reproduce the X-ray data of synthesized pyramidanes. The stationary points on the PES were located by full geometry optimization with calculations of force constants. XYZ-coordinates for reported structures are given in the Supporting Information (SI). Natural resonance theory (NRT) [25–27] analysis was carried out by the NBO 6.0 program package [28]. NRT calculations were performed for the corresponding model systems with R = H. NICS(1)$_{zz}$ indices [29] were calculated below the E'_4-bases, that is, on the opposite side to the apex. The views of the optimized geometries were generated using Chemcraft 1.8 program [30].

3. Results and Discussions

At the beginning, the simplest hydrogen-substituted model structures were studied. Only one model system $ClB[C_4H_4]$ **1** has symmetrical pyramidal structure as local minimum on the PES (Table 1). Other structures represent second- or third-order saddle points on the PES (Table 1) and their minima structures have distorted geometries (for the minima geometries of systems **4–9** as well as pyramidal nonminima structures **2–9;** see the SI). It is interesting that carbon-based systems **2** and **3** have housene-type structures as local minima (Figure 1). Small relative energy [0.8 kcal mol^{-1}, here and elsewhere – with zero point energy] of pyramidal (C_{4v}) **2** towards the C_s–minimum suggests flattened PES of $ClAl[C_4H_4]$, and there is a low-lying (0.9 kcal mol^{-1}) TS between two degenerated C_s–minima (Figure 2). Thus in case of $ClAl[C_4H_4]$ **2** there is a fast migration of ClAl fragment around C_4H_4 base providing pseudo-pyramidal structure. For housene system $ClGa[C_4H_4]$ **3** we also found corresponding TS with relative energy 9.8 kcal mol^{-1}.

Our previous work [14] showed the critical role of substituents for the stabilization of pyramidal structures, especially for the heavy ones with silicon and germanium

TABLE 2: Numbers of imaginary frequencies (NI) and relative energies towards closest minima (ΔE, kcal mol^{-1}) for pyramidal systems **1′**–**9′**.

Structure	E = B	E = Al	E = Ga
$ClE[C_4(SiMe_3)_4]$	**1′**, NI = 0	**2′**, NI = 0	**3′**, NI = 2, $\Delta E = 6.3$
$ClE[Si_4(SiMe^tBu_2)_4]$	**4′**, NI = 0	**5′**, NI = 0	**6′**, NI = 0
$ClE[Ge_4(SiMe^tBu_2)_4]$	**7′**, NI = 1, $\Delta E = 2.7$	**8′**, NI = 3, $\Delta E = 2.2$	**9′**, NI = 3, $\Delta E = 2.0$

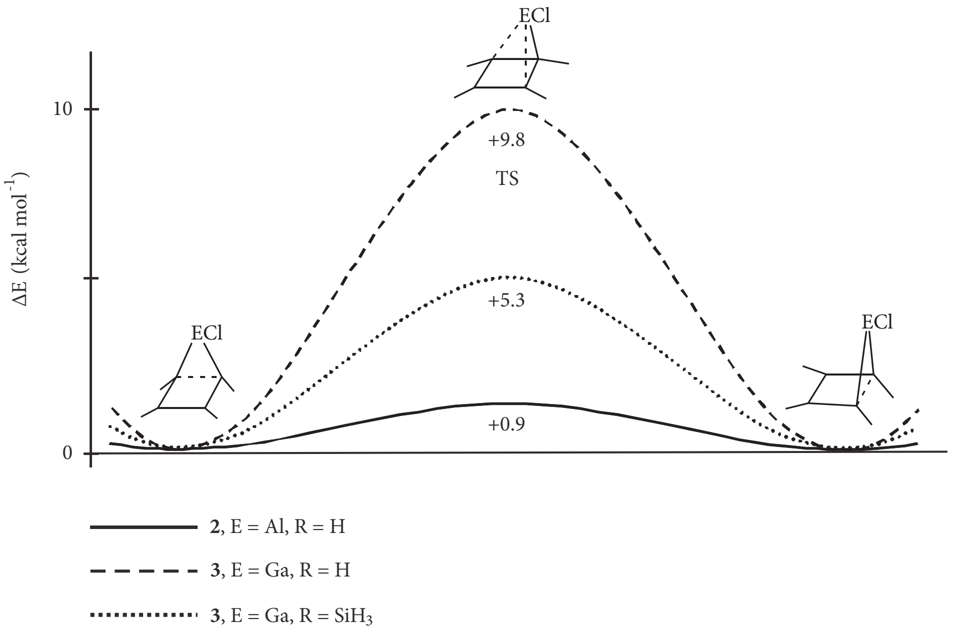
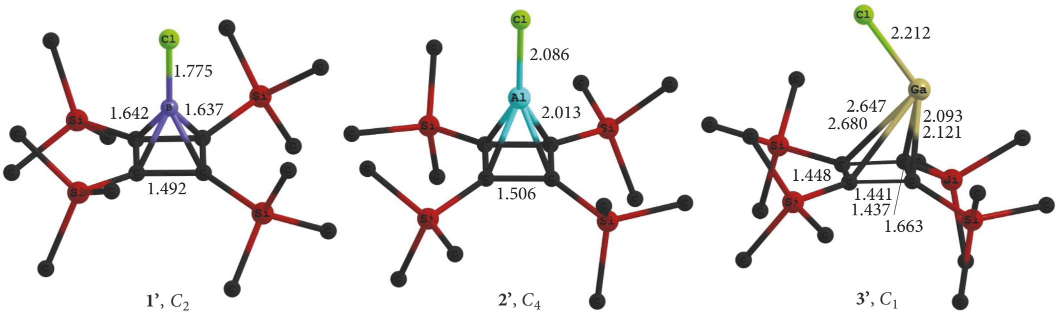


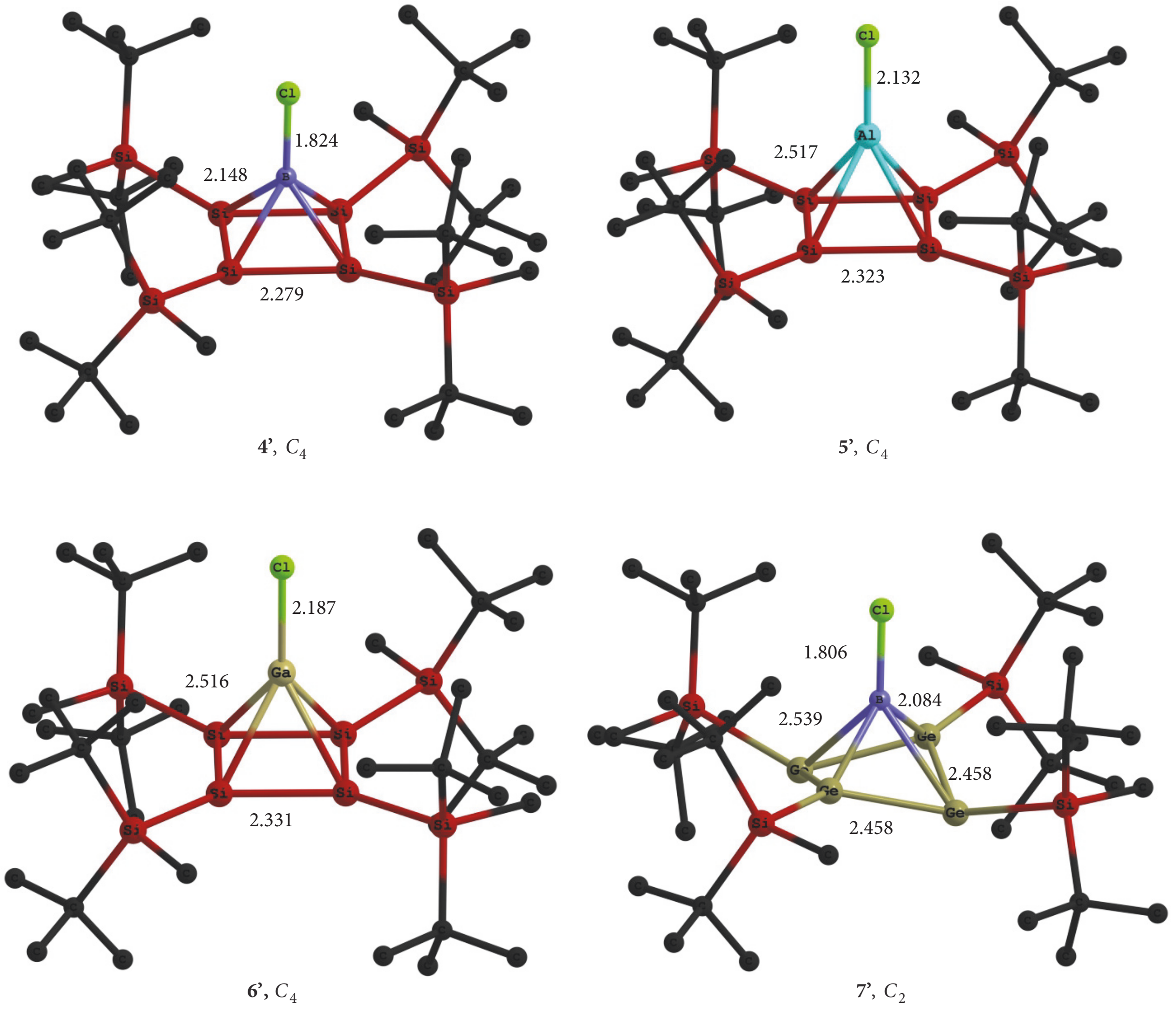
FIGURE 2: Energy profile for migration of ECl-fragment around the C_4R_4 basal ring for systems **2** and **3**.



1’, C_2 **2’**, C_4 **3’**, C_1

FIGURE 3: Optimized geometries (bond lengths are in Å) of minima structures **1′**–**3′**. Hydrogen atoms are omitted.

bases. Thus we performed the DFT calculations of compounds **1′**–**9′** with real substituents that are typically used in our experimental works (Table 2, R = $SiMe_3$, $SiMe^tBu_2$). As reported earlier [18], structure **1′** $ClB[C_4(SiMe_3)_4]$ has slightly distorted geometry with planar C_4-base. Calculated geometrical parameters (Figure 3) are in good agreement with the experimental X-ray data (C–C = 1.502, 1.493; B–C = 1.653, 1.643, 1.634; B–Cl = 1.766 Å) [18]. Geometrical trends of **1′** are in good agreement with the NRT calculations. Thus, NRT bond order for C–C bonds is 1.03 manifesting some little degree of the double bond character that corresponds to the calculated bond length value of 1.492 Å being intermediate between the standard single (1.54 Å) and double (1.34 Å) bond. Calculated $NICS(1)_{zz}$ index [29] of −7.9 for C_4 base indicates electron delocalization in basal cycle what keeps planarity of base and provides the pyramidal geometry for the system. For the comparison, $NICS(1)_{zz}$ for the benzene is −29.9 at the same level of theory. Pyramidal boron-carbon bonds in **1′** of 1.637 and 1.642 Å are longer than the sum of the single bond covalent radii of B and C atoms (1.60 Å) [31]. NRT bond order for B–C bonds is only 0.63. Nevertheless, B–C bonds are mostly covalent: the NRT covalent character is 58.8 %. The short length of B–Cl bond of 1.775 Å (the sum of the single bond covalent radii of boron and chlorine atoms is 1.84 Å) [31] well corresponds to the NRT bond order of 1.06 indicating some participation of double bonding.



4', C_4 **5'**, C_4

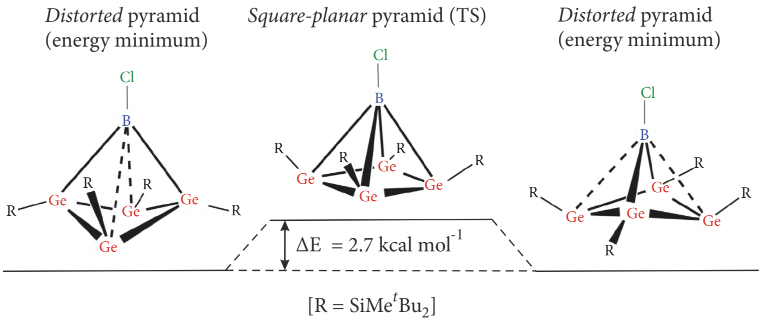
6', C_4 **7'**, C_2

FIGURE 4: Optimized geometries (bond lengths are in Å) of minima structures **4′**–**7′**. Hydrogen atoms are omitted.

Calculations of **2′** (E = Al) also predict stable pyramidal structure with symmetrical C_4-geometry (Figure 3). C–C bonds in **2′** of 1.506 Å are longer that in **1′**, but still intermediate between the standard single and double bonds, and have the greater NRT bond orders of 1.16. Aromaticity of the C_4-base is proved by the NICS(1)$_{zz}$ value of –10.9. Pyramidal Al–C bonds of 2.013 Å are only slightly longer than the sum of the single bond covalent radii of Al and C atoms (2.01 Å) [31]. NRT bond order for these bonds is 0.49, and the ionic character is 61.8 %. Apical ClAl-group has the Al–Cl bond value of 2.086 Å (the sum of the single bond covalent radii of Al and Cl atoms is 2.25 Å) [31], NRT Al–Cl bond order is 1.05, and the bond is by mostly ionic (NRT ionic character is 62.4 %).

In contrast with **1′** and **2′**, system **3′** (E = Ga) is represented by the housene-type structure, as shown in Figure 3. Symmetric pyramidal structure represents second-order saddle point (Table 2, for geometry see Figure S4 in the SI). As we mentioned above, there is a quite low-lying TS for the model housene structure **3** $ClGa[C_4H_4]$. Bulkier substituents might further decrease the energy of TS for such migrations [16]. The calculated barrier to migration is only 5.3 kcal mol^{-1} for H_3Si-substituted model system **3** $ClGa[C_4(SiH_3)_4]$, as shown in Figure 2. Such value is reasonable to consider a room temperature process for the migration of ClGa-group in **3′** that finally provides pseudopyramidal structure for it. Decrease in the migration barrier is accompanied by the decreasing of deviation angle of gallium towards C_4-base (see Figure 1): 102.7° for R = H, 99.3° for R = SiH_3, and 97.9° for R = $SiMe_3$.

Silicon-based structures **4′** (E = B, R = SiMe^{t}Bu$_2$), **5′** (E = Al, R = SiMe^{t}Bu$_2$), and **6′** (E = Ga, R = SiMe^{t}Bu$_2$) all have perfect pyramidal C_4-symmetry geometry at their energy minima points on the PES (Figure 4, Table 2) and are therefore good candidates for the synthetic realization. Si–Si bonds in **4′** of 2.279 Å are intermediate between the standard single (2.32 Å) [31] and double bond (2.14 Å) [32], and NICS(1)$_{zz}$ index of –9.6 approves electron delocalization in basal cycle of **4′**. Nevertheless NRT bond order of 0.97 indicate single Si–Si bonding in **4′**. Structures **5′** and **6′**



Scheme 1: Conformational interconversion in **7′**.

have Si–Si bonds of 2.32–2.33 Å corresponding to the single bond values. But NRT bond orders of 1.05 and 1.05 describe Si–Si bonds as having some degree of double bond character, and NICS(1)$_{zz}$ values of –10.2 and –10.9 indicate electron delocalization in Si$_4$-bases of **5′** and **6′**, respectively. As expected, pyramidal E–Si bonds in **4′**, **5′**, **6′** are longer than the sum of the single bond covalent radii of E and Si atoms (2.01, 2.42, 2.40 [31] Å for E = B, Al, Ga, respectively) and have low NRT bond orders of 0.69, 0.60, 0.59. Covalent characters calculated within the NRT are 75.6, 54.5, 61.9 % for the E–Si bonds (E = B, Al, Ga) in **4′**, **5′**, **6′**, respectively. E–Cl bonds in **4′**, **5′**, **6′** are shorter than the corresponding standard single bonds [31] by 0.02, 0.12, and 0.04 Å, respectively, and their NRT results point to a little extent of double bonding: the NRT bond orders are 1.02, 1.04, 1.00 for B–Cl, Al–Cl, and Ga–Cl, respectively.

Among the systems with the heaviest Ge$_4$-base there are no true pyramidanes: **7′** (E = B, R = SiMe^{t}Bu$_2$), **8′** (E = Al, R = SiMe^{t}Bu$_2$), and **9′** (E = Ga, R = SiMe^{t}Bu$_2$) minima structures all have distorted bases (like structure **7′** in Figure 4, for the minima structures **8′** and **9′** see Figure S3 in the SI). But among them the system ClB[Ge$_4$(SiMe^{t}Bu$_2$)$_4$] **7′** could be interpreted as effective pyramidal because of its low-lying (+2.7 kcal mol^{-1}) TS representing true square-pyramidal geometry (Figure S4 in the SI). Such phenomenon was previously observed in pentagermapyramidane Ge[Ge$_4$(SiMe^{t}Bu$_2$)$_4$] [15] and can be explained by the fast conformational interconversion between the folded minima and square-planar pyramidal TS (Scheme 1).

Four Ge–Ge bonds of 2.458 Å in minimum structure **7′** are longer than the standard single bonds (2.42 Å) [31] but have NRT bond order of 1.01 manifesting little contribution of the double bond character. The dihedral angle involving four Ge atoms is 26°. The TS structure characterized by planar Ge$_4$-base, shorter Ge–Ge bonds of 2.410 Å and NICS(1)$_{zz}$ index of –11.8. Two B–Ge bonds of 2.084 Å in minimum structure **7′** are close to the standard single bonds (2.06 Å) [31]. The other two B–Ge distances of 2.539 Å are much longer than the normal single bonds. B–Cl bond of 1.806 Å is shorter than the standard single bond (1.84 Å) [31], its NRT bond order is 1.00, and covalent character is 67 %.

Described structures could also be realized with other halogen atoms, and we calculated a structure BrB[C$_4$(SiMe$_3$)$_4$] **10′**, as such example. System **10′** corresponds to the energy minimum on the PES and has the same pyramidal geometry, as ClB[C$_4$(SiMe$_3$)$_4$] **1′** (Figure 3). C–C bonds in **10′** of 1.494 Å have NRT bond orders of 1.03. The NICS(1)$_{zz}$ index of –4.4 for C$_4$ base is nearly twice smaller than that for C$_4$ base in **1′** (–7.9). Pyramidal B–C bonds in **10′** of 1.637 and 1.640 Å are elongated comparing with single B–C bonds and have NRT bond orders of only 0.64. B–Br bond of 1.930 Å is shorter than the sum of the single bond covalent radii of boron and bromine atoms (1.99 Å [31]) and has the corresponding NRT bond order of 1.05 manifesting some extent of the double bonding.

4. Conclusions

According to our DFT calculations, synthetic realization of six pyramidal structures with the group 13 elements apical atom seems to be feasible: **1′** ClB[C$_4$(SiMe$_3$)$_4$] (experimentally realized), **2′** ClAl[C$_4$(SiMe$_3$)$_4$], **3′** ClGa[C$_4$(SiMe$_3$)$_4$] (effective pyramidal), **4′** ClB[Si$_4$(SiMe^{t}Bu$_2$)$_4$], **5′** ClAl[Si$_4$(SiMe^{t}Bu$_2$)$_4$], **6′** ClGa[Si$_4$(SiMe^{t}Bu$_2$)$_4$], and **7′** ClB[Ge$_4$(SiMe^{t}Bu$_2$)$_4$] (effective pyramidal). Structures with other halogen atoms could also be realized.

Data Availability

The geometry optimization data used to support the findings of this study are included within the supplementary information files.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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Supplementary Materials

Additional Supporting Information may be found online in the supporting information tab for this article. *(Supplementary Materials)*

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