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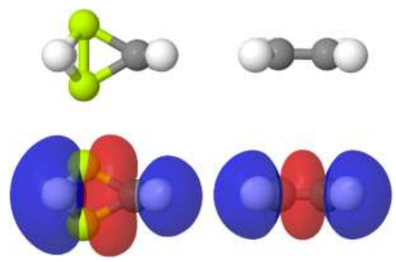


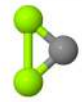
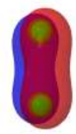
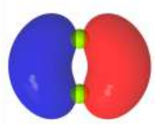
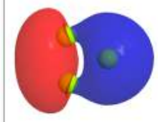
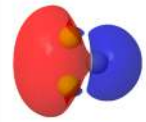
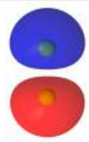
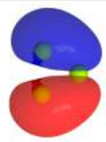
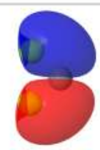
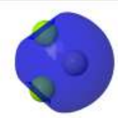
ABSTRACT: Controlled doping of active carbon materials (viz., graphenes, carbon nanotubes etc.) may lead to the enhancement of their desired properties. The least studied case of C/Be substitution offers an attractive possibility in this respect. The interactions of Be_2 with Be or C atoms are dominated by the large repulsive Pauli exchange contributions, which in turn offsets the attractive interactions leading to relatively small binding energies. The Be_2 dimer, e.g., after being doped inside a planar carbon network, undergoes orbital adjustments due to charge transfer and unusual intermolecular interactions and is oriented perpendicular to the plane of the carbon network with the Be−Be bond center located inside the plane. The present theoretical investigation on the nature of bonding in C/Be_2 exchange complexes, using state of the art quantum chemical techniques, reveals a sp^2 carbon-like bonding scheme in Be_2 arising due to the molecular hybridization of σ and two π orbitals. The perturbations imposed by doped Be_2 dimers exhibit a local character of the structural and electronic properties of the complexes, and the separation by two carbon atoms between beryllium active centers is sufficient to consider these centers as independent sites.

INTRODUCTION

The beryllium compounds are probably the least studied substances containing the second row elements.[1] Despite their unique chemical properties, not much work has been done so far to use such properties for practical applications. Part of the problem is due to the toxicity of the metal. There is also sufficient evidence for the carcinogenic properties of beryllium compounds causing lung cancer.[2] Beryllium, as one of the lightest atoms, on the other hand, offers an interesting possibility to functionalize carbon materials through carbon substitution. The carbon substitution by lithium, boron, nitrogen, and oxygen or their addition inside the carbon networks was extensively studied with the aim to replace heavy metals as catalysts.[3] The beryllium atom as well as beryllium dimer are interesting alternatives in search of new nanomaterials due to their unusual chemistry. For example, some of these Be-containing materials are promising alternatives for hydrogen storage media. Several microporous coordination polymers (MCPs) with Be-based secondary building units and metal organic framework (MOF) were synthesized with favorable adsorbent properties.[4−6] The direct Be substitution was also suggested as an efficient way to improve hydrogen adsorption.[7] There are two important bonds in such Be-substituted carbon networks that modulate their adsorption properties, viz. Be−C and Be−Be bonds. The Be−C bonding properties are not well studied so far, although a range of organoberyllium compounds are synthesized.[8−10] On the contrary, the Be−Be bond has drawn constant interest due to its unusual bonding properties.[11] The unusual character of beryllium compounds may be demonstrated from the properties of the Be_2 dimer. The dissociation energy of Be_2 (2.66 kcal/mol)[11] is an order smaller than the corresponding energy of covalently bonded dimer Li_2 (24.3 kcal/mol),[12] suggesting weak van der Waals type interactions in Be_2. The unusual nature of Be_2 dimer is further demonstrated in the bond distance of Be_2 dimer. The Be−Be bond distance (2.54 Å)[11] is shorter than that of Li_2 (2.67 Å) and also much shorter than weakly bonded Ne_2 (3.10 Å)[13] (characterized by typical nonbonding interactions of 0.08 kcal/mol). The bond distance of Be_2 shows that the dimer may be classified as one possessing significant covalent contribution, although energetically it is far from chemical bond characteristics of second row dimers *viz.* B_2 (R_e = 1.59 Å, D_o = 69.3 kcal/mol).[14]

The interaction with the third body (atom or molecular fragment) drastically changes the properties of Be_2 with several-fold increase of bonding energy. This phenomenon was

Table 1. Molecular Orbitals Involved in the Binding in Be_2, Be_3, and Be_2C

Be_2		Be_3		Be_2C	
Symmetry $C_{\infty h}$		Symmetry D_{3h}		Symmetry C_{2v}	
LUMO+1 π_u		LUMO a_2”		HOMO b_1	
LUMO π_u		HOMO e’		HOMO-1 a_1	
HOMO σ_u		HOMO-1 e’		HOMO-2 b_2	
HOMO-1 σ_g		HOMO-2 ·1’		HOMO-3 a_1	

observed in the case of Be_3 (Be atom as a third body) and Be_2C (C as the third body).[15] The Be_2 dimer, as a closed shell $\sigma_g^2\sigma_u^2$ complex of two interacting Be(^{1}S) atoms, is stabilized by the correlation energy due to low-energy 2p beryllium orbitals. The electronic ground state for Be_2 of $X^1\Sigma_g^+$ with the $\sigma_g^2\sigma_u^2$ configuration is accompanied by two deep low-lying excited electronic states: $1^3\Sigma_u^+$ with the $\sigma_g^2\sigma_u\sigma_g'$ configuration (T_e = 0.9 eV; T_e is the transition energy from the ground to the desired excited state) and $1^3\Pi_g^+$ resulting from $\sigma_g^2\sigma_u\pi_u$ configuration (T_e = 1.08 eV).[11] These configurations are isoelectronic with carbon possessing ground ^{3}P($2s^22p^2$), and low-lying excited ^{1}D and ^{1}S electronic states. Additionally, T_e’s between similar electronic states of C (1.263 eV for the C(^{3}P) to C(^{1}D) transition) and Be_2 are alike.[16]

The aim of this work is to determine the properties of the Be_2 dimer fragment after the substitution of a single carbon atom (by Be_2 dimer) in the sp^2 carbon network. The interactions of Be_2 with the rest of the system (the third body) modify its properties and impart new chemical properties to this center. Structures as well as the nature of bonding are being investigated using state of the art quantum chemical techniques. The newly evolved bonding characteristics of the Be_2 fragment in Be_3, Be_2C, $CH_2Be_2H_2$ (ethylene derivative), substituted aromatic compounds (benzene and naphthalene), and modified extended carbon materials (ovalene) was investigated. The computed geometric, orbital properties, charge distribution, and interaction energy decomposition results were not only found to be useful to enhance the present knowledge on Be−Be and Be−C chemical bonds but also could be used to predict the special chemical behavior of the Be center.

METHODS OF COMPUTATION

The computation of structural parameters of small molecules (Be_2, Be_3, Be_2C, and ethylene derivatives) were carried out using the Møller−Plesset second-order perturbation (MP2) methodology[17] with the aug-cc-pVTZ basis set for atoms.[18] For benzene and naphthalene derivatives the basis set was reduced to aug-cc-pVDZ.[19] The optimizations of Be doped ovalene ($C_{32}H_{14}$) structures were carried out at the density functional theory (DFT)[20] level using the B3LYP functional.[21−23] The test DFT calculations for smaller systems indicates that the method preserves the features observed at the MP2 studies. No symmetry constraints were imposed during the geometry optimizations. However, to model the planar extended structures, the position of the external ring was frozen in the geometry of $C_{32}H_{14}$. The computed energy values were further refined using single-point MP2-level energy calculations on the optimized structures with cc-pvdz basis set of atoms.

A hybrid variational−perturbational interaction energy decomposition scheme[24] was used to compute contributions of various energy terms in such interactions. The SCF interaction energy (ΔE^{HF}) is partitioned into first-order electrostatic ($\varepsilon_{el}^{(10)}$), Heitler−London exchange ($\varepsilon_{ex}^{(10)}$), and higher order delocalization (ΔE_{del}^{HF}) energy terms.

$$\Delta E^{HF} = \varepsilon_{el}^{(10)} + \varepsilon_{ex}^{HL} + \Delta E_{del}^{HF} \quad (1)$$

The electron correlation effects are taken into account by means of the MP2 theory. The $\varepsilon_{MP}^{(2)}$ interaction energy term, which includes the dispersion and correlation contributions to the Hartree−Fock components, is calculated in the supermolecular approach as the difference of MP2 energy corrections of the supermolecule and the monomers (eq 2).

$$\varepsilon_{MP}^{(2)} = E_{AB}^{(2)} - E_A^{(2)} - E_B^{(2)} \quad (2)$$

The energy terms on the right-hand side of eq 2 represent the difference between the MP2 and Hartree−Fock energies of the supermolecule (AB) and the monomers (A and B).

All the interaction energy terms are calculated consistently in the dimer-centered basis set and are therefore free from the basis set superposition error due to the full counterpoise correction.[25] The dispersion energy was also calculated directly by applying the expression for the second-order energy $\varepsilon_{disp}^{(20)}$. The atomic charges were computed using natural bond orbital (NBO).[26]

The geometry optimization calculations at MP2 and DFT/B3LYP were carried out using the Gaussian-09 code.[27] The interaction energy decomposition scheme implemented in the GAMESS code[28] was used for energy partitioning.[29] The molecular graphics have been generated using Jmol software.[30]

RESULTS AND DISCUSSION

a. Be_3 Bonding Properties. The Be_2 dimer is a weak complex due to interactions of closed 2s valence-shells of Be atoms. The third body, in the form of an additional beryllium atom, changes the orbital space organization and interactions lead to the D_{3h} triangle geometry of Be_3 with the significant dissociation energy. The Be−Be distance is reduced from 2.54 to 2.22 Å[11] due to such interactions. The inspection of molecular orbitals (MOs) indicates that the MO picture interpreted as a complex of Be_2 dimer and Be atom does not dramatically change the topological features. The $\sigma_g\sigma_u\pi_u$ orbitals of dimer could be easily projected onto three occupied orbitals (a_1', e', e') of the trimer (Table 1). The low-lying virtual π_u orbital, being transformed into a_2'' within the D_{3h} symmetry representation, does not directly take part in the bonding at the HF level. However, this effect significantly stabilizes the beryllium trimer when the correlation energy is included.

$$\Psi_4(a_1') = 2s(Be_1) + 2s(Be_2) + 2s(Be_3)$$
$$\Psi_5(e') = 2p_x(Be_1) + 2s(Be_2) - 2s(Be_3)$$
$$\Psi_6(e') = 2s(Be_1) + [2p_y - 2s](Be_2) + [2p_y - 2s](Be_3) \quad (3)$$

The simplified molecular orbital composition of valence atomic components (eq 3), in contrast to the beryllium dimer, indicates the increasing role of atomic p orbitals. They are responsible for significant covalent bond contribution in the bonding.

The interaction energy decomposition for the Be_2 + Be system indicates the high values of interaction energy components compared to the total interaction energy. The attractive interaction energy terms offset the extremely high exchange repulsion contribution ε_{ex}^{HL} (Table 2), resulting in small bonding energy. The delocalization energy ΔE_{del}^{HF} (responsible for induction interactions) constitutes the largest attraction term. It is totally quenched by the exchange interaction energy. The electrostatic $\varepsilon_{el}^{(10)}$ and dispersion energies $\varepsilon_{disp}^{(20)}$, although smaller in value, are very important in the final balance of bonding energy. The results of the interaction energy partitioning thus indicate the importance of covalent forces to the overall bonding mechanism. The large values of energy components canceling the small total interaction energy constitutes a major characteristic feature of molecular bonding of Be clusters. The large and dominating Pauli exchange repulsion term canceling attractive contributions is also a typical characteristics for the Be−Be bonding.

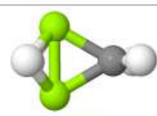
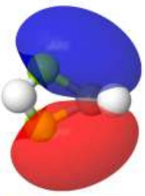
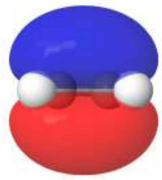
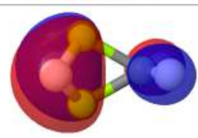
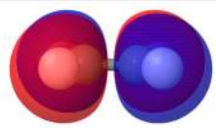
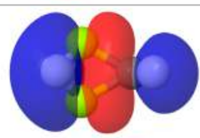
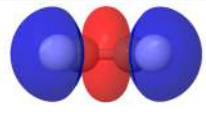
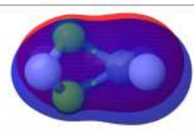
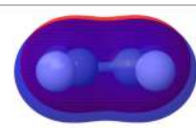
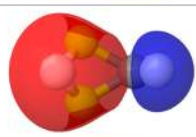
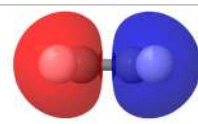
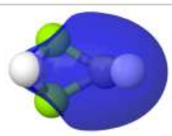
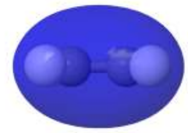
Table 2. Interaction Energy Decomposition Terms for Be_2, Be_3, and Be_2C Interacting Complexes (Energies in kcal/mol)

	Be_2	Be_3	Be_2C
interacting fragments	Be + Be	Be_2 + Be	Be_2 + C(^{1}S)
$\varepsilon_{el}^{(10)}$	−10.0	−43.7	−205.1
ε_{ex}^{HF}	24.8	104.0	486.9
ΔE_{del}^{HF}	−10.6	−72.2	−363.7
ΔE^{HF}	4.2	−11.8	−81.8
$\varepsilon_{dis}^{(20)}$	−7.7	−28.3	−59.1
$\varepsilon_{MP}^{(2)}$	−5.1	−30.3	−28.3
ΔE^{MP2}	−0.9	−21.8	−110.1
$\Delta E^{CCSD(T)}$	−0.9	−21.7	−145.7

b. Nature of the Chemical Bond in the Be_2C Complex. The Be_2C complex is formed with an atomization energy of 129.1 kcal/mol. The lowest energy structure of the $^1A_1$ (C_{2v} symmetry) electronic state possesses the T-shaped geometry and is characterized by Be−Be: 2.117 Å and Be−C: 1.584 Å bond distances. These results are in good agreement with extended CCSD(T) (2.068 and 1.598 Å) and CASSCF (2.087 Å and1.607 Å) calculations.[11] It is to be noted that the inclusion of electronic correlation is essential for the proper determination of the electronic ground state structure. The lower level of theory leads to the wrong prediction of geometry of the ground electronic state.[11−13] The Be−Be bond in Be_2C is much shorter than the one in the Be_2 dimer; however, the composition and topology of the orbitals are preserved (compared to the Be_2 dimer) and are well visible as molecular orbital components of Be_2C. The σ_g, σ_u, π_u, and π_u' orbitals of the Be_2 fragment form MOs with 2s, $2p_x$, $2p_y$, and $2p_z$, of carbon, respectively (Table 1). The HOMO of π character stabilizes the structure by forming three center-two electron (3c2e) delocalized bond. The other bonds are also delocalized and cover the whole molecule. The NBO atomic charges (C: −1.611; Be 0.805 electron) indicate atomic charge separation in the molecule. The Be−Be distance in Be_2C correlates with Be_2^+ (2.211 Å) rather than Be_2 (2.54 Å).[11] This confirms that the computed charge distribution pattern leads to significant ionic contribution to the C−Be bond. Similar to the Be_3 case, the intermolecular interactions are dominated by the exchange repulsion term ε_{ex}^{HL} (Table 2). The largest attractive contribution is of induction origin (ΔE_{del}^{HF}, delocalization term); however, the electrostatic contribution is also significant. The absolute values of interaction energy contributions are large with respect to the total Hartree−Fock (HF) interaction energy. It is an indication that chemical manipulation on the bonding properties will greatly influence the final energy. The already attractive HF energy is further enhanced by the correlation contribution.

c. Ethylene vs $CH_2Be_2H_2$ Derivative. The structure of the $CH_2Be_2H_2$ complex matches closely with CH_2CH_2. The Be−Be axis is perpendicular to the ideal plane defined by carbon and hydrogen atoms and the midpoint X of the Be−Be bond (Figure 1S, Supporting Information). The molecular orbital pictures of substituted ethylene and its parent molecule are very similar (Table 3) with the HOMO having π character. The perturbations in the ethylene skeleton, imposed by the C/Be_2 substitution, do not change the basic topological features of the MOs and the correspondence between the orbitals is obvious and easily tractable within the D_{2h} to C_{2v} transformation (Table

Table 3. Valence Molecular Orbitals for $CH_2Be_2H_2$ Complex and Complementary Ethylene Molecules

$CH_2Be_2H_2$		CH_2CH_2	
Symmetry C_{2v}		Symmetry D_{2h}	
HOMO b_1		HOMO b_{3u}	
b_2		b_{3g}	
a_1		a_g	
b_2		b_{2u}	
a_1		b_{1u}	
a_1		a_g	

3). The XH_2 angle (114.9°) is very close to one in the complementary $-CH_2$ fragment (111.2°) and in ethylene (117.4°). The orbitals in the valence space of the Be_2 dimer in the complex (σ_g, σ_u, π_u, π'_u) transform from σ_u, π_u, π'_u into the $\sigma\pi^2$ configuration (Figure 1). This transformation is analogous to the hybridization of 2s, $2p_x$, $2p_y$ atomic orbitals in carbon. The σ_u orbital, not involved in the hybridization, corresponds to the orthogonal p_z orbital in the sp^2-hybridized carbon. The center of molecular hybrids ($\sigma\pi^2$) is located at the midpoint X of the Be−Be bond. The additional σ_g (LUMO) is not included in the bonding scheme and constitutes the reactive orbital on the Be−Be axis with no analogue available in pure ethylene. Due to the substitution, the character of double C═C bond is preserved and in the X═C case is represented by $\pi(b_{3u}\rightarrow b_1)$ and $\sigma(a_g\rightarrow a_1)$ orbitals.

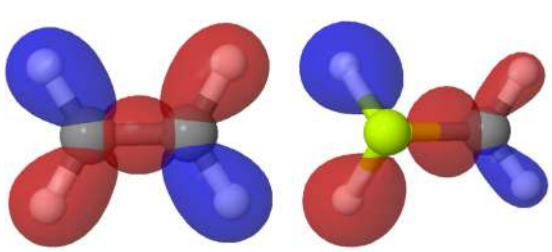

a b

Figure 1. Ethylene and $C_2Be_2H_2$ combined HOMO σ orbitals corresponding to the sp^2 hybridization ($\sigma\pi^2$ in case of beryllium derivative): (a) ethylene b_{3g}, a_1, b_{1u}; (b) $C_2Be_2H_2$ b_2, a_1, a_1.

The electronic population analysis, due to the delocalized character of molecular orbitals, is very sensitive to the method of computation. The NBO population analysis indicates the local character of perturbation associated with the C/Be_2 substitution. The charges on hydrogens in the CH_2 group are similar to that in the ethylene case (Figure 1S, Supporting Information). The value of $-Be_2H_2$ to $-CH_2$ charge transfer (−0.924 electron) should be treated with a caution considering the rather low dipole moment of the molecule of 2.323 D. The much shorter Be−Be distance of 1.718 Å with respect to the Be_2 dimer (2.54 Å) and Be_2^+ cation (2.11 Å) indicates large involvement of beryllium atoms in the bonding mechanism. The very short Be−Be distance compares well with deeply bound excited states of Be_2^+ and suggests the importance of contribution from low-lying electronic states to the bonding in studied systems.[31,32]

d. Substituted Aromatic Systems. The C/Be_2 and $(C/Be_2)_2$ substitutions were studied in benzene and naphthalene. In all the cases, substitution leads to the same structural modification preserving the planar ring, and the Be_2 axis being perpendicular to the plane of the complex (Figure 2). The

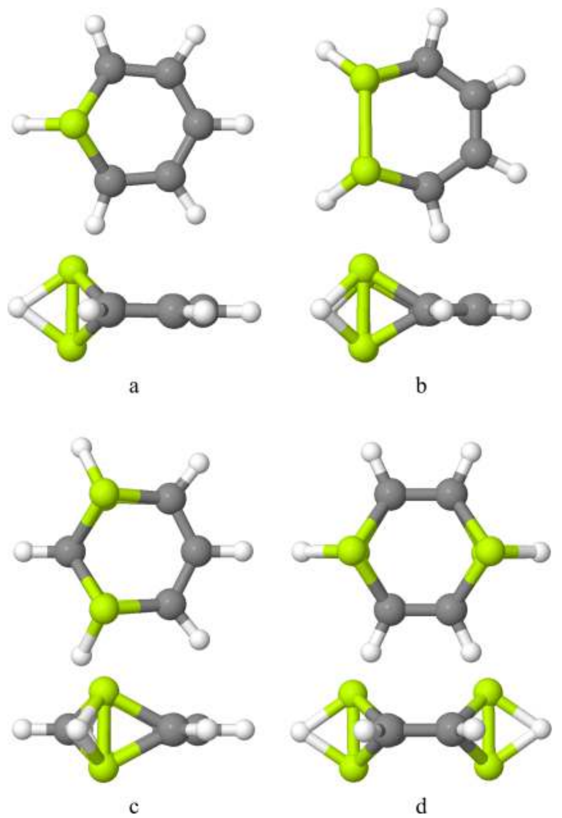


Figure 2. Top and side views of single (a) and double ((b) ortho, (c) meta, (d) para) Be_2 derivatives of benzene.

midpoint (X) of the Be−Be bond lies inside the plane of the ring and constitutes the center of the orbitals related to Be_2 bonding. The hydrogen atom closest to Be_2, complements the skeleton of the parent benzene molecule. The Be−Be distance in all the studied structures is close to 1.7 Å, indicating a similarity of ethylene involvement in Be_2 in bonding. The molecular orbital picture corresponds to the proposed molecular model of $\sigma\pi^2$ hybridization (Figure 3). The

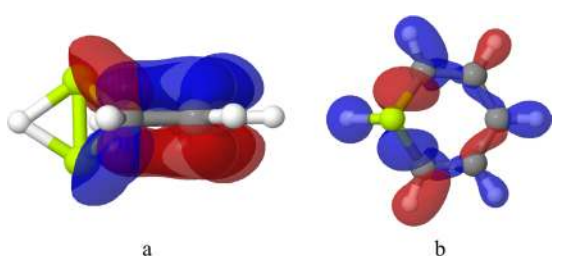


Figure 3. Combined (a) three HOMO π orbitals (side view) and (b) three HOMO σ orbitals covering the beryllium bond in the plane of the molecular ring (top view) in $C_5Be_2H_6$ benzene derivative.

combined picture of three molecular orbitals located in the plane of carbon skeleton (Figure 3) covers two C−X σ bonds and one X−H bond (X represents the center of the Be−Be bond). The combined molecular orbital picture of the three HOMO π orbitals indicates the involvement of the Be_2 orbital in the overall π bond system. The NBO atomic charge on each beryllium atom amounts to 0.941 electron. When C is substituted in two different locations of the benzene ring, they also have NBO charges close to this value (ortho, 0.512; meta, 0.970; para, 0.849 electron). The total dipole moment of C/Be_2 substituted benzene (calculated with aug-cc-pVTZ basis set) amounts to 0.712 D. The insertion of the second Be dimer does not change the overall picture of the bonding scheme and only little perturbation in comparison to the singly substituted benzene is observed. The substituted naphthalene molecule follows the same structural trend regardless of the position of substitution (Figure 2S, Supporting Information). Molecular orbitals and atomic charges are almost the same as those observed in the benzene case. The differences between isomers were also insignificant.

e. Extended Carbon Systems. The functionalization of carbon materials may improve their desired properties. The hydrogen storage on pure carbon materials is restricted due to very weak interactions with molecular hydrogen. The substitution of carbon atom or decoration of material with foreign chemical groups provides the direct way to enhance the adsorption properties. The investigated structures in the present section are based on the ovalene model (an extended graphene-like carbon material) (Figure 4). The carbon

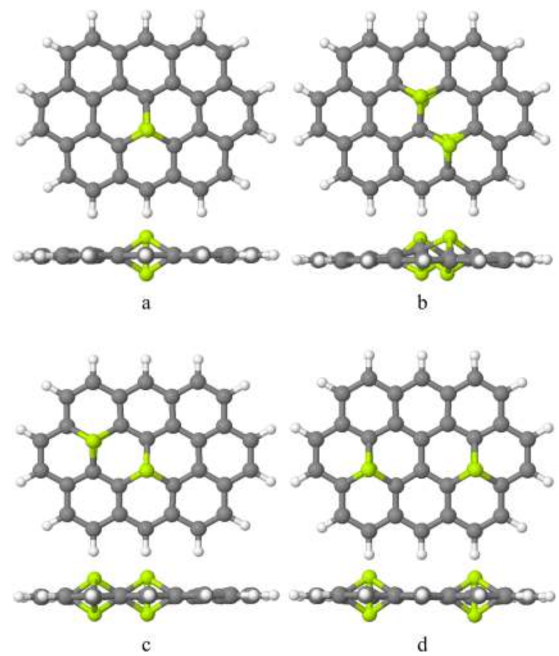


Figure 4. Structures for single and double C/Be_2 substitutions in the $C_{32}H_{14}$ ovalene base: (a) single C/Be_2 substitution; double $(C/Be_2)(C/Be_2)$ substitutions with (b) Be_2−C−Be_2, (c) Be_2−C_2−Be_2, (d) Be_2−C_3−Be_2 carbon separation.

substitution by Be_2 leads to a similar geometrical picture like the previously discussed ethylene and aromatic compounds. The Be_2 axis is perpendicular to the plane of the carbon skeleton with the midpoint of Be−Be bond lying inside the plane. Further carbon/beryllium substitution is possible and all probable isomers of Be_2−C_n−Be_2 (n = 1−4) are considered here. Regardless of the carbon separation with respect to the beryllium centers, the structural features of these isomers correspond to the general characteristic of the fragment (vertical Be_2 moiety). Only the isomer with a single carbon separation is slightly perturbed from the perfect perpendicular geometry of Be_2. All Be−Be distances in such dimers with doubly substituted centers are within 0.015 Å with respect to the singly substituted moiety. The C−Be bonds are also very similar in these dimers (despite different metal center positions), indicating little influence of the border effects due to the frozen external carbon ring. The picture of molecular orbitals observed for the extended $C_{31}H_{14}Be_2$ complex (Figure 5) is similar to the aromatic compounds. The HOMO π orbital

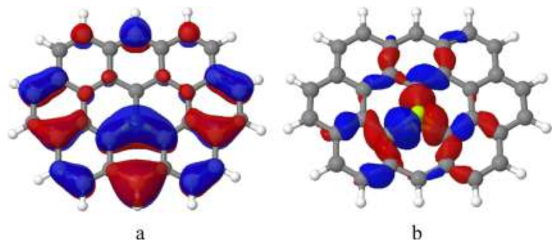


Figure 5. Π HOMO (a) and combined three σ HOMO molecular orbitals (b) (perspective view) of $C_{31}H_{14}Be_2$ localized on the beryllium dimer.

above the Be_2 center constitutes part of the extended delocalized π system. The σ combined orbitals representing the $\sigma\pi^2$ arrangement are also dipped in the sea of delocalized orbitals. The Be−Be distance in all the cases is close to 1.73 Å. The comparison of all considered complexes indicates that perturbations due the Be_2 insertion in the ring are almost independent when Be_2 centers are separated by at least two carbon atoms. The substitution leads to the local modification of properties of original molecules as may be observed by the atomic charge distribution. The beryllium NBO charge was approximately 1.15 electron in single Be_2 as well as in double substitution. More importantly, the characteristics of substitution centers (geometrical or electronic) is also similar to one observed in the single substitution. The difference in properties disappears for Be_2 centers for distances larger than two carbon atoms. The local character of substitutions indicates the existence of independent active centers.

CONCLUSIONS

The doping of active carbon or nanocarbon materials is a promising direction for controlling their physical and chemical properties. In this work, the beryllium dimers were studied as potential active centers in the carbon body. Be_2 represents a weakly bonded complex, with low-lying excited electronic states. These states, when activated by interaction with the "third body", lead to complexes of much higher bonding energy. The bonding in complexes results from the competition between the highly repulsive Pauli exchange energy (ε_{ex}^{HL}) and the attractive interaction energy terms ($\varepsilon_{el}^{(10)}$, ΔE_{del}^{HF}, $\varepsilon_{disp}^{(20)}$). The values of separate contributions are comparable to those characterizing chemical bonds. Although in $CH_2Be_2H_2$, the Be−Be distance is significantly shortened due to the interactions with the environment, the molecular orbital picture of the valence space ($\sigma_g\sigma_u\pi_u\sigma_g$) is preserved and constitutes the basis for the MO formation in larger systems. The substitution of single carbon by the pair of beryllium atoms does not destroy planarity and the aromaticity of the carbon network. The inclusion of Be_2 in the place of carbon preserves the symmetry characteristics of complex with axis of Be_2 being perpendicular to carbon network with the midpoint X of Be−Be bond located in the original carbon position (i.e., plane of the ring). The position of hydrogen (or hydrogens), originally attached to the replaced carbon is also preserved. This phenomenon was observed in all studied systems where substituted carbon possessed the sp^2 character. The midpoint X of Be_2 may be considered as a "pseudo sp^2 carbon atom" with $\sigma\pi^2$ orbital organization of valence orbitals—an analogue to the atomic sp^2 case. The molecular orbital pictures, presented for ethylene, benzene, naphthalene, and ovalene derivatives, confirm the proposed model. The σ_g orbital of Be_2 is included in the sea of π molecular orbitals of conjugated molecules (in analogy to the p_z atomic orbital in carbon systems). The perturbations due to the doping were found to possess the local character and may be considered in larger systems as chemically active centers. The positive atomic charges on beryllium atoms are large and shortening of the bond can be attributed to the Be_2^+ fragment. The results of population analysis should be treated with caution, however, due to the extensively delocalized character of electronic density.

ASSOCIATED CONTENT

Supporting Information

Optimized structures of $CH_2Be_2H_2$ and CH_2CH_2 and views of Be_2-substituted benzene and naphthalene derivatives.

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Notes

The authors declare no competing financial interest.

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