**Ternary CE$_2$Ba$_2$ (E = As, Sb) Clusters: New Pentaatomic Planar Tetracoordinate Carbon Species with 18 Valence Electrons**

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Received: 25 March 2022 / Accepted: 15 July 2022 / Published online: 26 July 2022
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**Abstract**

18-valence-electron (ve) rule is one important guide for us to design planar tetracoordinate carbon (ptC) species. Using the “polarization of ligands” strategy, the new pentaatomic ptC species CE$_2$Ba$_2$ (E = As, Sb) with 18 ve are designed in this work. Computer structural searches and high-level calculations reveal that the ptC CE$_2$Ba$_2$ (E = As, Sb) species are global minima (GMs) on the potential energy surfaces, whose C center is coordinated by the interspaced E and Ba atoms. CE$_2$Ba$_2$ (E = As, Sb) are also kinetically stable. Chemical bonding analyses reveal that the ptC core is stabilized by two localized C-E σ bonds, one delocalized five-center two-electron (5c-2e) σ bond and one delocalized 5c-2e π bond. One π and three σ bonds collectively conform to the 8-electron counting, which determines the stability of ptC CE$_2$Ba$_2$ (E = As, Sb) species. Interestingly, the delocalized 2π and 2σ electrons render the ptC systems π/σ double aromaticity. Additional 10 electrons contribute to peripheral lone pairs of E and E-Ba bonding.

**Keywords** Planar tetracoordinate carbons (ptCs) · 18ve counting · Pentaatomic cluster · Global minimum · Aromaticity

**Introduction**

Exploring the bonding capacity of carbon beyond the classical tetrahedral concept, has been a interesting and challenging subject in chemistry for decades. Compared with the tetrahedral configuration, planar tetracoordinate carbon (ptC) structure is unstable with the higher energy in most cases. In 1968, Monkhorst proposed a ptC configuration as transition state in the interconversion of enantiomers[1]. Just 2 years later, Hoffmann et al. put forward the ingenious strategies to stabilize the ptC systems, based on the deep bonding analyses for a hypothetical planar $D_{4h}$ CH$_4$[2]. Since Schleyer and coworkers predicted the first ptC local minimum (1,1-dilithiocyclopropane) in 1976[3], a variety of ptC, planar pentacoordinate carbon (ppC), and planar hexacoordinate carbon (p6C) species were theoretically designed/predicted or experimentally observed in gaseous phase using anion photoelectron spectroscopy, which each possesses 17 or 18ve[23–27]. According to the isoelectronic principle, the ptC clusters, CE$_4$$_2^-$ (E = Al, Ga, In, Ti), CGa$_2$Si$^-$, and CAL$_3$E (E = P, As, Sb, Bi), were theoretically predicted[28–30]. However, 18ve counting is
not a prerequisite. Indeed, several pTC species have been reported, which go beyond the 18-electron rule[31–36]. Anyway, 18ve counting is still a nice guide to design some new pTC species. Very recently, using the “polarization of ligands” strategy, Merino and coworkers predicted a series of pTC clusters with 18ve, which can be formulated as $\text{M}_m\text{CE}_2^p$ ($E =$ S-Te, $M =$ Li-Cs, $m =$ 2, 3 and $p = m-2$)[15]. Now, the open question is: Is there any undiscovered pentaatomic pTC clusters with 18ve? The answer seems to be “yes.”

Herein, we have tried to find the correct combination towards a pTC system as the global minimum. Based on the “polarization of ligands” strategy, the pTC $\text{CE}_2\text{M}_2$ ($E =$ N-Bi; $M =$ Be-Ba) species can be considered. However, only pTC $\text{CE}_2\text{Ba}_2$ ($E =$ As, Sb) clusters with 18ve are the global mimima at the density functional theory (DFT) level. As we all know, DFT method is reliable for theoretical design [37–41]. $\text{CE}_2\text{Ba}_2$ ($E =$ As, Sb) possess the perfect rhombus structures with $D_{2h}$ symmetry, whose pTC center is coordinated in-plane by the interspaced E and Ba atoms. The pTC $\text{CE}_2\text{Ba}_2$ ($E =$ As, Sb) clusters are established as the global mimima (GMs) via unbiased computer searches. Bonding analyses indicate that the pTC core in cluster 1/2, has one $\pi$ and three $\sigma$ bonds, collectively conforming to the “octet rule.” The octet rule (eight-electron rule) seems to be universally applicable for the pTC clusters. Peripheral lone pairs (LPs) and E-Ba bonding in cluster 1/2 involves 10 electrons. The results obtained in this work will complete the series of the pentaatomic pTC species with the 18ve. It is further confirmed that “polarization of ligands” is an effective strategy for expanding pTC clusters.

**Methods**

The GM structural searches for $\text{CE}_2\text{Ba}_2$ ($E =$ As, Sb) clusters were carried out using the Coalescence Kick (CK) algorithm[42–44] at the PBE0/Lanl2DZ level[45]. A total of 4000 points (2000 singlets and 2000 triplets) were explored on the potential energy surface for each species. Low-lying candidate structures were subsequently reoptimized at PBE0-D3/def2-TZVPP level[46, 47]. Vibrational frequency analyses were done at the same levels to ascertain their nature as true minima. In addition, the identified GM structures and four low-lying isomers were also optimized at the B3LYP-D3/def2-TZVPP level[48, 49]. To refine the energetics, single-point CCSD(T)[50–52] calculations were performed for top five structures at their PBE0-D3/def2-TZVPP and B3LYP-D3/def2-TZVPP geometries.

To get the data of Wiberg bond indices (WBIs) and natural atomic charges of the $\text{CE}_2\text{Ba}_2$ ($E =$ As, Sb) clusters, we performed the natural bond orbital (NBO)[53] analyses at the PBE0-D3/def2-TZVPP level. Canonical

![Scheme 1](image)
molecular orbital (CMO) and adaptive natural density partitioning (AdNDP)[54] analyses were done to explore the bonding characteristics. Nucleus-independent chemical shifts (NICSs)[55] were calculated at PBE0/def2-TZVPP, to quantitatively probe the π and σ aromaticity. The orbital compositions were analyzed by the Multiwfn program[56]. All calculations of electronic structures were done by the Gaussian 09 package[57]. Molecular structures, canonical molecular orbitals (CMOs), and AdNDP bonding patterns were visualized using the CYLview and Molekel programs [58, 59].

Results and discussion

**Design of ptC CE2Ba2 (E = As, Sb)**

CA142− is the most representative pentaatomic cluster with 18ve, which possesses perfect D4h symmetry. As shown in Scheme 1, using “polarization of ligands” strategy, we can obtain three ptC CE2M2 series, based on different degree of polarization of ligands. Some of ptC CE2M2 (E = C, Si, Ge, Sn, Pb; M = B, Al, Ga, In, Tl) clusters have been reported, such as CSi2Al2, CGe2Al2, CSi2Ga2, and CGe2Ga2. Very recently, the ptC CE2M2 (E = S, Se, Te; M = Li, Na, K, Rb, Cs) clusters were investigated systematically by Merino et al.[15], which are all true ptC GMs on their potential energy surfaces. It should be noted that the degree of polarization of ligands in (a) is smallest, while that of (c) is biggest. Here, we attempted to stabilize ptC by using a combination of nitrogen group elements and alkaline earth metal atoms as ligands. Thus, an interesting issue arises: Are the ptC CE2M2 (E = N, P, As, Sb, Bi; M = Be, Mg, Ca, Sr, Ba) clusters GMs? To answer above question, two major computational efforts have been made. The first effort is to examine ptC CE2M2 (E = N, P, As, Sb, Bi; M = Be, Mg, Ca, Sr, Ba) clusters, which adopt D2h and C2v structures as true minima. As shown in Table S1, there are 12 ptC species are minima without the imaginary frequencies, which include C2v CN2M2 (M = Be, Mg), D2h CE2M2 (E = P, As; M = Sr, Ba), and D2h CE2M2 (E = Sb, Bi; M = Ca, Sr, Ba).

As depicted in Fig.S1, the WBIC-Be and WBIC-Mg are only 0.09 and 0.03, respectively, indicating there is little covalent bonding between C and Be/Mg in CN2M2 (M = Be, Mg). In addition, both C and Be/Mg carried the positive charges (C +0.42/ +0.38 |e|, Be +0.67 |e|, Mg +0.79 |e|), suggesting there are only Coulomb repulsion between them. Thus, the C

![Fig. 1 Optimized global minimum (GM) structures 1, 2 of CE2Ba2 (E = As, Sb) clusters at the PBE0-D3/def2-TZVPP level. Bond distances (in Å), Wiberg bond indices (WBIs; blue color), and natural atomic charges (in |e|; red color) are shown](image)
atoms in CN₂M₂ (M = Be, Mg) are hardly to be considered as the true ptCs. The second effort is to perform the GM searches. For D₂h CE₂M₂ (E = P, As; M = Sr, Ba) and D₂h CE₂M₂ (E = Sb, Bi; M = Ca, Sr, Ba), the systematic isomers searches and high-level calculations indicate that only ptC CE₂Ba₂ (E = As, Sb) are true GMs.

**Structures and stability**

The optimized GM structures 1, 2 of CE₂Ba₂ (E = As, Sb) at PBE0-D3/def2-TZVPP level are shown in Fig. 1. The four low-lying isomers (nB−nD) are depicted in Fig. 2, along with their relative energies at the single-point CCSD(T)/def2-TZVPP level with zero-point energy (ZPE) corrections at PBE0-D3. Cartesian coordinates for top five lowest lying structures are listed in Table S2 (ESI†). The GM clusters 1, 2 are 4.85 and 19.50 kJ·mol⁻¹ more stable than their closest competitors, respectively. In terms of energetics, CSb₂Ba₂ is particularly well defined on its potential energy surfaces. The GM structures and low-lying isomers contain a tetracoordinate carbon center, except isomer 2E (Fig. 2).

As depicted in Fig. 1, the C-As bond distance in 1 is 1.84 Å, while the C-Ba distance is 2.49 Å. Although C-As/C-Ba bonding is polar, the C-As/C-Ba single bond has an upper bound of 1.96/2.71 Å based on covalent atomic radii[60]. Therefore, the C-As bonding in 1 is quite strong, probably greater than single bond. interestingly, the As-Ba bonding is also substantial and being close to a half bond. Wiberg bond indices (WBIs) and natural population analysis (NPA) charges offer valuable bonding information. The WBI data for clusters 1, 2 are also shown in Fig. 1. For CE₂Ba₂ (1), the C center has robust bonding with its coordinating As ligands (WBIs: 1.34), which possesses the partial double bond properties. The C-Ba link has relatively small WBIs (0.36). For the periphery, 1 has substantial E-Ba bonding (WBIs: 0.48), which is close to...
half a bond. In terms of NPA charges, the C center carries a negative charge of $-1.54 \text{|e|}$ for 1, while the Ba, As ligands possess the charge of $+1.16$ and $-0.39 \text{|e|}$, respectively, due to the difference of electronegativity. The WBIs and NPA charges in 2 are similar with those of 1, there are only a few minor differences.

Global searches of the potential energy surfaces of CE$_2$Ba$_2$ (E = As, Sb) indicate that ptC structures 1 and 2 as the GM structures have good thermodynamic stabilities (Fig. 2). For experimental characterization, the dynamic stability of clusters is as important as the thermodynamic stability. To probe the dynamic stability of CE$_2$Ba$_2$ (E = As, Sb) (1 and 2), Born–Oppenheimer molecular dynamics (BOMD) simulations[61] were performed at the PBE0/def2-SVP level, for 50 ps at room temperature (300 K). The root-mean-square deviations (RMSDs) during these BOMD simulations are the reliable evaluation indicators for the kinetic stability. As depicted in Fig. 3, the average RMSDs of clusters 1, 2 are relatively small (0.31 and 0.20 Å), suggesting that the ptC CE$_2$Ba$_2$ (E = As, Sb) clusters possess good kinetic stabilities, being robust against decomposition or isomerization.

**Chemical bonding and aromaticity**

To elucidate the stability of ptC CE$_2$Ba$_2$ (E = As, Sb) clusters, it is essential to perform chemical bonding analyses. Since the essence of bonding is similar in ptC CE$_2$Ba$_2$ (E = As, Sb) species (1, 2), herein, we only use 1 as an example. The CAs$_2$Ba$_2$ cluster has 18 valence electrons. All the occupied CMOs and their compositions of CE$_2$Ba$_2$ (E = As, Sb) are shown in Table S3-S4.

AdNDP is an important analysis approach for chemical bonding, which is an ingenious extension of NBO method. AdNDP analyses recovers typical Lewis bonding elements (LPs and two-center two-electron (2c-2e) bonds) and novel delocalized nc-2e ($n \geq 3$) bonds. As shown in Fig. 4, the AdNDP analyses provide a relatively simple and intuitive bonding picture for the ptC CAs$_2$Ba$_2$ cluster. Figure 4(a) shows that there are two lone pairs (LPs) of two As atoms. As Fig. 4(b) shown, there is one three-center two-electron (3c-2e) As-C-As π bond, with $\text{ON} = 1.80 \text{|e|}$, which is one non-bonding orbital in nature, because there is no contributions of C. In other words, it contributes little to the stability of the system. On the periphery of the cluster,
there are two Ba-As-Ba (3c-2e) σ bonds, with ON = 2.00 |e| (Fig. 4(c)). The ptC CAS₂Ba₂ (1) cluster has a relatively rigid peripheral E₂Ba₂ ring, which is interconnected via two 3c-2e Ba-E-Ba σ bonds. As a comparison, there is only one delocalized 4c-2e σ bond for the peripheral Al₄ ring in CAI₄²⁻. As shown in Fig. 4(d), there are two localized C-As (2c-2e) σ bonds and one delocalized 5c-2e σ bond. In addition, there is one 5c-2e π bond, with ON = 2.00 |e|, as shown in Fig. 4(e).

Interestingly, the Ba atoms participate in global π framework via their 5d AOs (by 4%). Although the most important contribution is from As-C-As, the contribution of two Ba atoms seems to be cannot be neglected. Thus, one delocalized π bond together with one σ bond rendered the ptC clusters 2π/2σ double aromaticity, following the (4n+2) Hückel rule.

As shown in Fig. S2, cluster 2 has similar bonding patterns with 1, three σ and one π bonds around the ptC core.

As depicted in Fig. 5, the π/σ double aromaticity of ptC clusters 1, 2 is independently confirmed via the NICS calculations. Systems with negative NICS values are considered aromatic. All NICS(1) (from −7.06 to −15.50 ppm) and NICS(0) (−6.53 and −9.18 ppm) are negative at PBE0/def2-TZVPP, which are calculated at 1 Å above the ptC center, and above 1/0 Å of the center of a C-E-Ba triangle. The NICS values suggest that ptC clusters 1, 2 truly possess π and σ double aromaticity, in line with bonding analyses.

In order to facilitate future experimental characterization, the IR spectrums of the ptC clusters 1 and 2 were simulated theoretically at the PBE0-D3/def2-TZVPP level (see Fig. S3). As shown in Fig. S3, the absorption peak at 493 cm⁻¹ of CAS₂Ba₂ (1), mainly originates from C-Ba anti-symmetry stretching vibration. The peak at 989 cm⁻¹ originates from its anti-symmetry C-As stretching vibration. The other absorption peaks are mainly generated by coupled vibrations. The calculated IR spectra of CSb₂Ba₂ turned out to be similar with CAS₂Ba₂. All absorption peaks of CSb₂Ba₂ are redshifted slightly, due to the large mass number of Sb.

Conclusions

We have designed two planar tetracoordinate carbon (ptC) clusters, CE₂Ba₂ (E = As, Sb), which are GMs via unbiased structural searches and high-level quantum chemical calculations. Chemical bonding analyses suggest that the ptC CE₂Ba₂ (E = As, Sb) clusters have one π and three σ bonds around the ptC core, which make the carbon center conform to the octet rule. Additional ten electrons contribute to peripheral lone pairs of E and E-Ba bonding. One delocalized π bond together with one delocalized σ bond endow the 2π and 2σ double aromaticity. The bonding pattern is ideal for these ternary ptC clusters, justifying their 18-electron counting.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s00894-022-05229-1.

Author contribution Fang-Lin Liu: all calculations, data analysis, and manuscript preparation. Jin-Chang Guo: supervision, manuscript preparation, conceiving the problem, data analysis, and correction.

Funding This work was supported by the National Natural Science Foundation of China (22173053 and 21873058).

Code availability No new codes have been created. Existing codes were utilized and quoted correctly.

Declarations

Conflict of interest The authors declare no competing interests.

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