Chemical Physics Letters 835 (2024) 140999

Contents lists available at ScienceDirect

Chemical Physics Letters

journal homepage: www.elsevier.com/locate/cplett

Research paper

# Carbon nanobracelets

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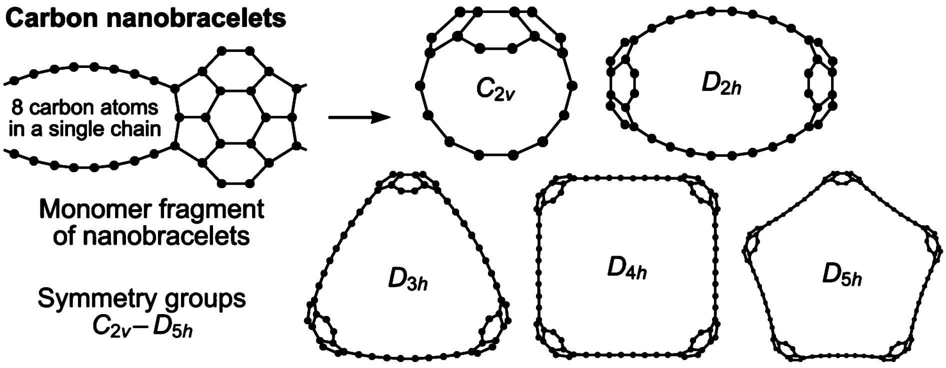
## GRAPHICAL ABSTRACT



## HIGHLIGHTS

- Cyclic molecules with alternate aromatic regions and double carbon chains are studied.
- Alternation of short and long bond in chains of carbon nanobracelets is observed.
- All considered carbon nanobracelets have the highest possible symmetry.
- Difference in properties of nanobracelets with even and odd monomer number is found.
- Hydrogen at aromatic region enhances the redistribution of electron density within monomer.

## ARTICLE INFO

Dataset link: https://doi.org/10.17632/jx6b58kfyy

*Keywords:*
Carbon macromolecules
Carbyne
DFT calculations
Carbon chain
Cyclic polymer

## ABSTRACT

Carbon-based cyclic molecules with alternating polycyclic regions and double carbon chains referred to as carbon nanobracelets are studied using spin-polarized density functional theory (DFT) calculations with PBE functional. Optimized structure of considered nanobracelets consisting of 1–5 identical monomers with and without hydrogen atoms at the edge of polycyclic regions is found to have highest possible symmetry and bond length alternation in chains. Nanobracelets consisting of odd number of monomers have lower HOMO energy, greater HOMO-LUMO gap and greater bond length variation in the carbon atomic chains than nanobracelets with even number of monomers.

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https://doi.org/10.1016/j.cplett.2023.140999
Received 15 September 2023; Received in revised form 17 November 2023; Accepted 21 November 2023

## 1. Introduction

Carbon atomic chains have been produced from graphene nanoribbons [1–5], and carbon nanotubes [6,7], by removal of carbon atoms under electron irradiation in high-resolution transmission electron microscope. Due to their transport properties carbon chains are candidates for application in spintronic [8–11] and electronic [11–14] devices. A wide set of 2D carbon networks which contains atomic carbon chains has been considered and synthesized via various approaches (See Ref. [15] for a review).

Moreover not only single carbon chains are possible. According to DFT calculations zigzag graphene nanoribbon with width of one hexagon (i.e. two zigzag atomic rows) is unstable and decays with formation of double carbon atomic chains [3]. Thus polyaromatic hydrocarbon molecules, polymers and 2D systems with acen-like regions (i.e. one hexagon wide) in a structure can transform after hydrogen removal into objects which contains double carbon atomic chains. This prediction is confirmed by a set of experimental studies and atomistic simulations. Cyclic polyaromatic molecules with double carbon chains are observed to form due to hydrogen loss at laser evaporation of carbon nanobelts [16]. Formation of double carbon chains rarely occurs at etching of graphene nanoribbon under electron irradiation [1,3]. Formation of triple carbon chains is also predicted at heating of zigzag graphene nanoribbon with width of two hexagons [17]. Recently formation of 1D nanoobject with alternating double carbon chains and polycyclic regions from a graphene nanoribbon with alternating regions which are one and three hexagons wide due to hydrogen loss under electron irradiation has been proposed [18].

In parallel with the studies of double carbon chains formation methods to produce cyclic hydrocarbons have been elaborated [19,20] (see also Ref. [21] for a review). The progress in the studies of objects with double carbon chains formed due to hydrogen loss and the synthesis of cyclic hydrocarbons allows us to propose that synthesis of cyclic molecules with double carbon chains will be realized in the nearest future. In the present paper we use density functional theory (DFT) calculations to consider structure and electronic properties of carbon-based cyclic molecules with alternating polycyclic regions and double carbon chains referred to as carbon nanobracelets.

## 2. Methods

Optimization of structure was performed with the spin-polarized DFT calculations using PBE functional [22]. The Priroda code [23] which allows to considerably reduce the computational time and therefore to study large molecules was used for the all-electron calculations. The adequacy of Priroda code has been previously confirmed by comparison of structural characteristics and energetics of oxygen interaction with small metal clusters [24] and energy of oxygen adsorption on different carbon nanostructures [25] with the values obtained using other DFT-based codes. The energy-optimized extended Gaussian basis set of triple-n quality of the large component and the corresponding kinetically balanced basis for the small component were used [26]. Energies of carbon nanobracelets were calculated taking into account zero point energy.

It has been discussed that thermally-assisted-occupation (TAO) DFT [27,28], is more appropriate for consideration of cyclic molecules since using of a conventional DFT with semilocal functionals may exhibit strong static correlation effects [29]. TAO-DFT method is tested by comparison [28] with an accurate M06-L functional [30]. We compare for the smallest considered nanobracelet the results obtained by PBE functional implemented in the Priroda code with the results obtained by M06-L functional implemented in NWChem code [31] and found that both functionals give the same bond lengths with the difference in the HOMO-LUMO energy gap about 0.1 eV. Thus we believe that using of PBE functional is appropriate for consideration of the proposed nanobracelets.

To obtain by DFT calculations optimized structures of the considered large molecules which contain long flexible carbon atomic chains starting coordinates should be sufficiently close to the final coordinates. For this reason, the starting coordinates for DFT calculations have been prepared by following several steps. Initial coordinates made by hand have been optimized by molecular mechanics [32]. Then PM3 optimization with high-symmetry conservation implemented in MOPAC2016 [33] has been performed to obtain the starting coordinates for the optimization by Priroda code.

Since symmetry breaking is possible for cyclic molecules (see, for example Ref. [34]) the symmetry of the nanobracletes after the DFT-based structure optimization was determined by the algorithm [35] implemented in the free WebMO server software [36,37]. All optimized nanobracelets have only positive vibrational frequencies therefore the optimized structures correspond to the true minima. The lists of vibrational frequencies and optimized coordinates are openly available in *Mendeley Data*, see Ref. [38].

## 3. Carbon nanobracelet properties

### *3.1. Structure and energy*

Two kinds of the carbon nanobracelets without and with hydrogen atoms attached to the polycyclic regions with the number $n_m$ of identical monomers (the polycyclic region with double chains on one side) $n_m = 1$–$5$ are considered. The structure of polycyclic regions of nanobracelets is taken the same as the structure of such regions of 1D carbon nanoobjects with double chains formed from graphene nanoribbon with alternating width under electron irradiation [18]. Optimized structures of all considered nanobracelets are presented in Figs. 1 and 2 for the nanobracelets without and with hydrogen atoms, respectively. All considered nanobracelets conserve the highest possible symmetry after the DFT-based optimization. For all considered nanobracelets without hydrogen atoms we check that using of starting coordinates obtained without high-symmetry conservation (which correspond to structures with the broken symmetry) leads at DFT optimization to the same high-symmetry structure. The singlet ground state has a lower energy than the triplet ground state for all nanobracelets considered. The energy differences between triplet and singlet ground states are listed in Table 1. Note that the molecule with a polycyclic region with the other structure and double chains ($n_m = 1$) has been obtained in the experiment [16].

According to Figs. 1 and 2 angles between nearest chains connecting polycyclic regions tend to be 90°: for number of monomers $n_m < 4$ chains are bent outwards, for $n_m = 4$ chains are straight, for $n_m > 4$ chains are bent inwards.

Radiuses $R$ of the considered nanobracelets without hydrogen atoms linearly depend on the number of monomers $n_m \geq 2$ and behave as $R(n_m) = (1.66+2.65n_m)$ Å within the standard deviation 0.03 Å. Radiuses $R$ of the considered nanobracelets with hydrogen atoms linearly depend on the number of monomers $n_m \geq 2$ and behave as $R(n_m) = (1.55 + 2.67n_m)$ Å within the standard deviation 0.02 Å.

In the chains of nanobracelets, an alternation of bond lengths is observed. In order to characterize the magnitude of this alternation, we determined the amplitude of bond length variations in chains according to [9,10] as

$$\delta = \frac{1}{2}\left|\frac{1}{n_e}\sum_{j=1}^{n_e}(d_{2j-1} + d_{n-(2j-1)}) - \frac{1}{n_0}\sum_{j=1}^{n_0}(d_{2j} + d_{n-2j})\right|, \tag{1}$$

where $d_i = |\mathbf{r}_i - \mathbf{r}_{i+1}|$ is the bond length between $i$th and $(i+1)$-th atoms in the chain, $n$ is the number of atoms in the chain, natural numbers $n_e = (n+2)/4$ and $n_0 = n/4$ (the integer part is taken). In this formula, terminal bonds connecting chain to the polycyclic fragment are not taken into account.

Variation of the bond lengths in the chain $\delta$ assessed by Eq. (1) for the considered carbon nanobracelets with $n_m \geq 2$ correspond to the

**Table 1**

Calculation details for the considered nanobracelets with number of monomers $n_m$ from 1 to 5: symmetry after optimization, circumscribed sphere radius (from the center of mass), short and long lengths in the chain without terminal bonds connecting to the polycyclic fragment, variation of the bond lengths in the chain $\delta$, energy of the nanobracelet per monomer $E/n_m$ relative to the lowest energy nanobracelet with 5 monomers in singlet ground state, dipole moment, HOMO-LUMO energy gap $E_{\text{H-L}}$, the absolute values of HOMO and LUMO energies, and differences between triplet and singlet ground states $E_T - E$.

| Number of monomers $n_m$ | Symmetry[a] | Radius (Å) | Short lengths (Å) | Long lengths (Å) | $\delta$ (pm) | $E/n_m$ (eV) | Dipole (D) | $E_{\text{H-L}}$ (eV) | $-E_{\text{HOMO}}$ (eV) | $-E_{\text{LUMO}}$ (eV) | $E_T - E$ (eV) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Nanobracelets without hydrogen atoms | | | | | | | | | | | |
| 1 | $C_{2v}$ | 4.10 | 1.25 | 1.33 | 7.8 | 4.7057 | 0.73 | 0.7057 | 5.57 | 4.87 | 0.6113 |
| 2 | $D_{2h}$ | 6.93 | 1.25–1.26 | 1.31 | 6.0 | 0.6884 | 0 | 0.2790 | 5.32 | 5.04 | 0.0453 |
| 3 | $D_{3h}$ | 9.63 | 1.24–1.25 | 1.31–1.32 | 6.9 | 0.0291 | 0 | 0.6292 | 5.64 | 5.01 | 0.4258 |
| 4 | $D_{4h}$ | 12.26 | 1.25 | 1.31–1.32 | 6.2 | 0.0063 | 0 | 0.2761 | 5.36 | 5.09 | 0.1762 |
| 5 | $D_{5h}$ | 14.88 | 1.25 | 1.31–1.32 | 6.6 | 0 | 0 | 0.5003 | 5.51 | 5.01 | 0.3083 |
| Nanobracelets with hydrogen atoms | | | | | | | | | | | |
| 1 | $C_{2v}$ | 4.02 | 1.25 | 1.33 | 7.8 | 4.9620 | 0.62 | 0.6116 | 5.34 | 4.73 | 0.2586 |
| 2 | $D_{2h}$ | 6.87 | 1.25–1.26 | 1.31–1.32 | 5.9 | 0.6979 | 0 | 0.3348 | 5.12 | 4.78 | 0.1716 |
| 3 | $D_{3h}$ | 9.59 | 1.25 | 1.31–1.32 | 6.5 | 0.0477 | 0 | 0.5886 | 5.39 | 4.80 | 0.3711 |
| 4 | $D_{4h}$ | 12.23 | 1.25–1.26 | 1.31–1.32 | 6.0 | 0.0020 | 0 | 0.3578 | 5.15 | 4.79 | 0.2209 |
| 5 | $D_{5h}$ | 14.90 | 1.25 | 1.31–1.32 | 6.2 | 0 | 0 | 0.4798 | 5.27 | 4.79 | 0.3697 |

[a] The tolerance with what the symmetry group was detected was less than 0.010 for nanobracelets without hydrogen atoms and less than 0.023 for nanobracelets with hydrogen atoms.

range $\delta$ = 5.9–6.9 pm and decreases in oscillating manner: maximum values for an odd number $n_m$ of monomers in a carbon nanobracelet and minimum values for even number $n_m$ of monomers (see Table 1). The oscillation of bond length variation in the chains with the number of monomers in a cyclic polymer has been found previously for carbon rings [34]. On average, variation $\delta$ is about 0.2 pm larger for carbon nanobracelets without hydrogen atoms. The calculated values of the bond length variation are in excellent agreement with the previous DFT calculations $\delta$ = 6 pm [9] and 5.5 pm [10] for straight atomic carbon chains composed of 8 atoms attached to zigzag graphene edges. Note that the bond length variation in chains is greater than the bond length variation $\delta$ = 3.9 pm assessed by Eq. (1) for the Kekule-type structure predicted for the ground state of (6,0) carbon nanotube [39].

Energy of the nanobracelet per monomer $E/n_m$ relative to the lowest energy nanobracelet with 5 monomers decreases almost exponentially with the number $n_m$ of monomers; each next value of the relative energy is an order of magnitude smaller than the previous one. Thus we believe that the structural parameters of the monomer and electronic properties of the nanobracelets do not noticeably change with a further increase of the number $n_m$ of monomers.

### 3.2. Electronic properties

In order to gain a comprehensive understanding of the electronic properties of the carbon nanobracelets the dipole moment, charge density distribution, and the energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were calculated. The calculated dipole moment, HOMO and LUMO energies and HOMO-LUMO energy gap for the considered carbon nanobracelets are listed in Table 1.

The main consequence of molecular symmetry is that only molecules belonging to the groups $C_n$, $C_{nv}$, and $C_s$ may have a permanent electric dipole moment [40]. The smallest nanobracelet have $C_{2v}$ point group, and its dipole moment is nonzero. For the carbon nanobracelets with the higher symmetry $D_{2h}$–$D_{5h}$, the calculated dipole moment is zero within an accuracy of 0.01 D. This is confirmed the determined symmetry of the nanobracelets.

The energy difference (gap) between the HOMO and LUMO levels $E_{\text{H-L}}$ is a crucial factor in understanding the carbon nanobracelet stability. For both carbon nanobracelets without and with hydrogen atoms the HOMO-LUMO energy gap $E_{\text{H-L}}$ slightly decreases with increase of the number of monomers $n_m$ in oscillating manner analogously to variation of bond length in chains described in Section 3.1. Maximum values of the gap are found for an odd number $n_m$ of monomers in a nanobracelet and minimum values are found for an even number $n_m$ of monomers. Mean values of $E_{\text{H-L}}$ are almost the same for nanobracelets without and with hydrogen: (0.48 ± 0.20) eV and (0.47 ± 0.13) eV, respectively. Average amplitudes of oscillations are 0.34 eV (without hydrogen) and 0.22 eV (with hydrogen). Thus, the amplitude of oscillations is 0.12 eV higher for carbon nanobracelets without hydrogen atoms.

The absolute values of HOMO and LUMO energies in Table 1 indicate that oscillations of the gap $E_{\text{H-L}}$ with the number of monomers $n_m$ are related mainly with oscillations of the LUMO energy. Nanobracelets with hydrogen atoms at the edge of polycyclic regions have lower absolute values of both HOMO and LUMO energies in comparison with the pure carbon nanobracelets. Thus it is possible to assume that the nanobracelets with hydrogen would easier donate electron, while the pure carbon nanobracelets would easier accept electron.

HOMO and LUMO for the smallest carbon nanobracelet consisting of one monomer without hydrogen atoms and with hydrogen atoms are visualized and shown in Fig. 3a and b, respectively. The visualization of HOMO and LUMO for nanobracelets consisting of 2–5 monomers is analogous. For nanobracelets without hydrogen atoms (Fig. 3a), the LUMO electron density is distributed over polycyclic regions with five- and six-membered rings that form a conjugating system. Thus, the polycyclic region can act as an electron acceptor in chemical reactions. The HOMO electron density is localized near the carbon chain, so they can act as electron donor. Hydrogen presence in nanobracelets does not lead to the changes in HOMO and LUMO electron density. Nanobracelets consisting of even number of monomers have lower HOMO-LUMO energy gap and therefore higher HOMO level can be somewhat more chemically active than nanobracelets consisting of even number of monomers.

By examining the charge density distribution, the spatial arrangement and localization of electrons within the carbon nanobracelets can be determined (see Fig. 4a and b for the carbon nanobracelets without and with hydrogen atoms, respectively). For the carbon nanobracelets without hydrogen atoms an excess of electron density on the carbon atomic chains is found to be −0.04$e$, where $e$ is the elementary charge, whereas the polycyclic regions are characterized by a lack of electron density (+0.04$e$), see Fig. 4a. The accumulation of electron density on the carbon atomic chains is probably related with the presence of triple bonds. Presence of hydrogen atoms in carbon nanobracelets at edges of polycyclic regions results in a diminished electron density within the polycyclic regions and an augmentation of electron density along the carbon atomic chains, see Fig. 4b. Specifically, the lack of

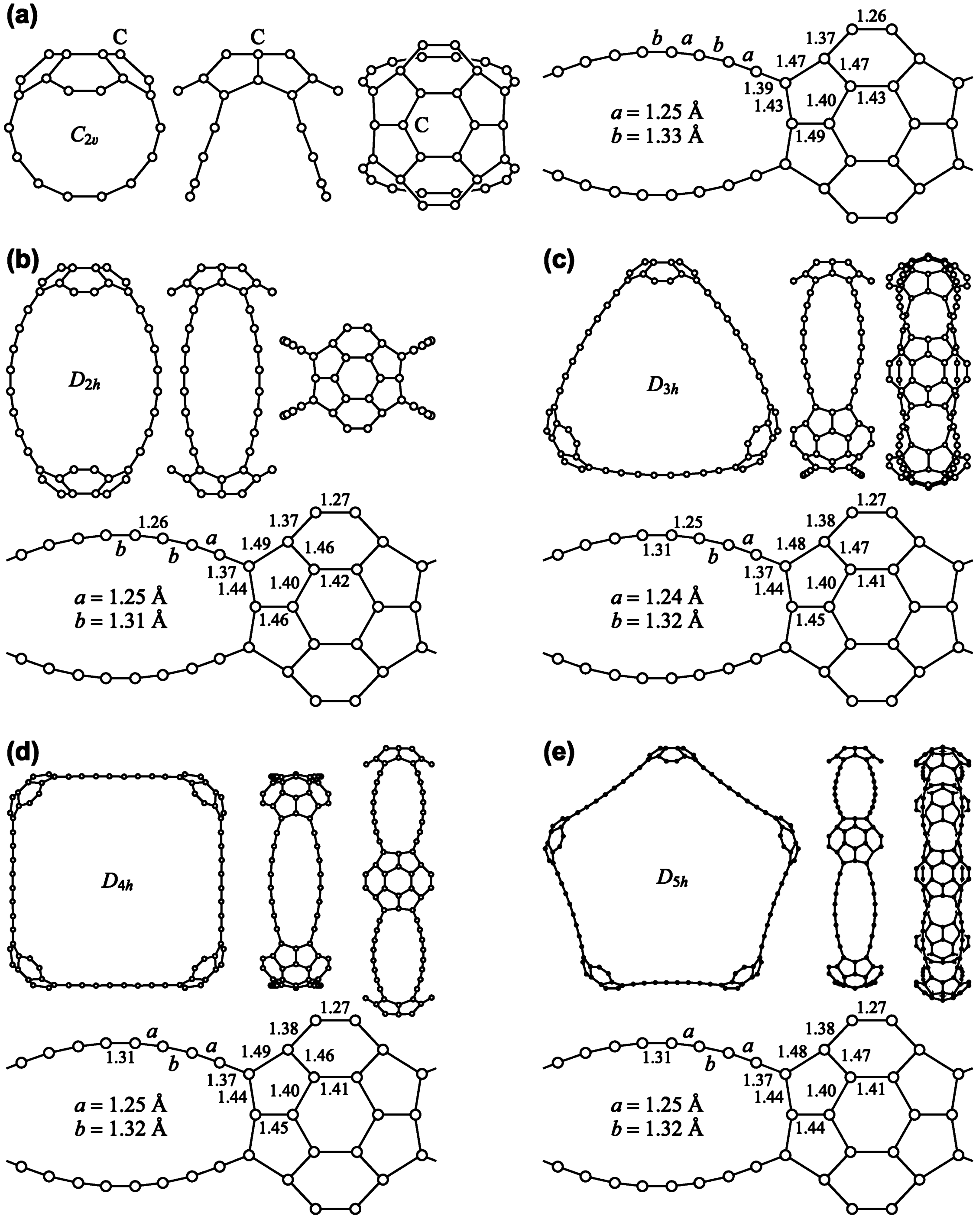

**Fig. 1.** Carbon nanobracelets without hydrogen atoms composed of $n_m$ monomers from 1 to 5 (a)–(e), respectively. Each nanobracelet is shown in three projections. Corresponding point symmetry groups $C_{2v}$–$D_{5h}$ of the nanobracelets are indicated. Bond lengths are shown in monomer fragment of the nanobracelet below projections.

electron density on the polycyclic fragments escalates from $+0.04e$ to $+0.06e$, while there is a concomitant increase in the excess of electron density for the carbon chains from $-0.04e$ to $-0.05e$. Given this data, it can be deduced that the presence of hydrogen atoms enhances the redistribution of electron density within nanobracelets between the atomic chains and the polycyclic fragments. It should be noted that the number of monomers in the carbon nanobracelets does not significantly influence on the charge density distribution. This confirms the conclusion below based on the energy calculation that electronic properties of the nanobracelets do not noticeably change with the increase of the nanobracelet size.

## 4. Conclusions and discussion

The possibility of synthesis of carbon-based cyclic molecules with alternating polycyclic regions and double carbon chains referred to as carbon nanobracelets is proposed. The spin-polarized DFT calculations with PBE functional implemented in the Priroda code are used to study structure, symmetry, energy and electronic properties of nanobracelets consisting of identical 1–5 monomers with and without hydrogen atoms at the edge of polycyclic regions. For all considered nanobracelets the highest possible symmetry and alternation of short and long bonds in the chains is observed for the optimized structure. The structural

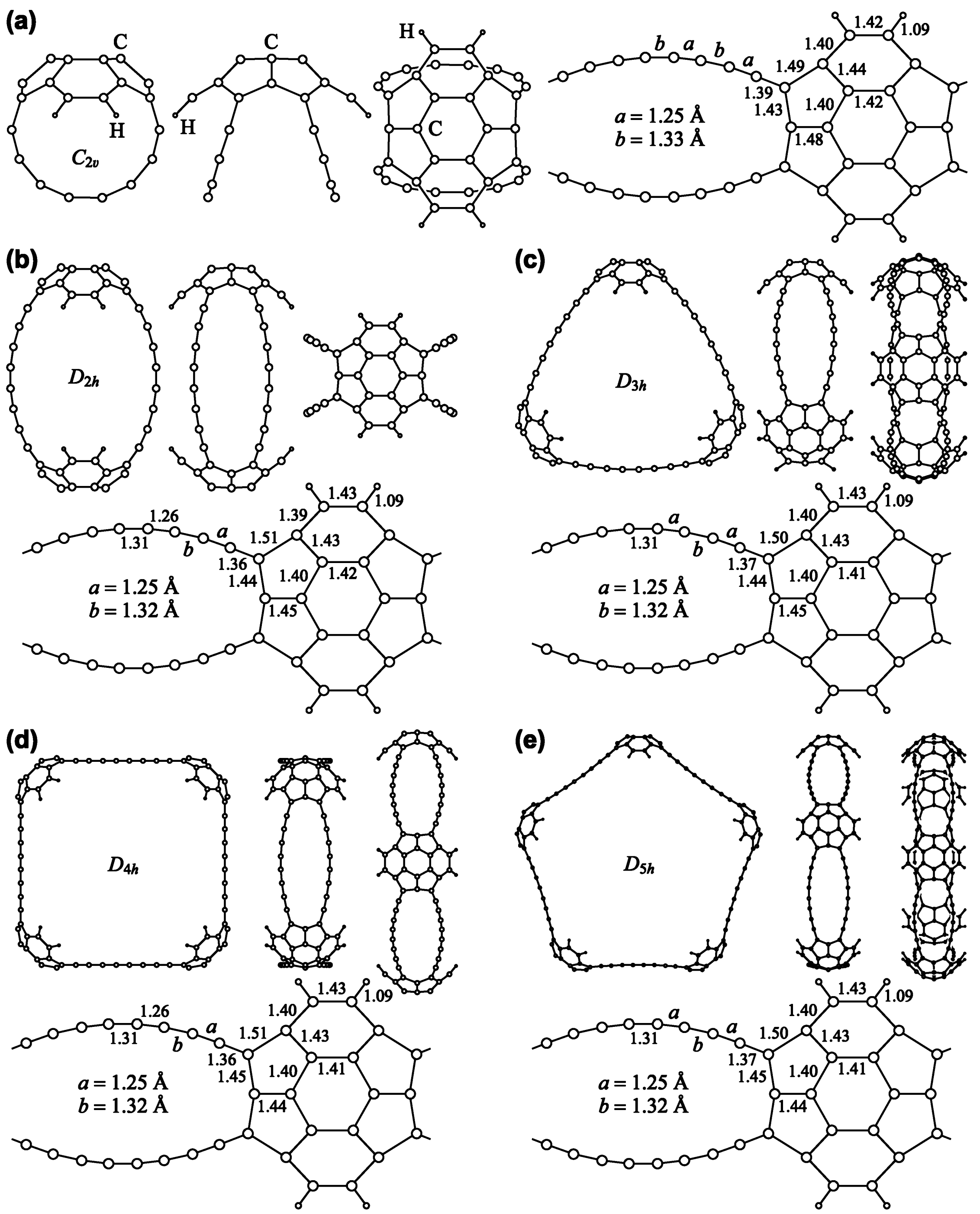

**Fig. 2.** Carbon nanobracelets with hydrogen atoms composed of $n_m$ monomers from 1 to 5 (a)–(e), respectively. Each nanobracelet is shown in three projections. Corresponding point symmetry groups $C_{2v}$–$D_{5h}$ of the nanobracelets are indicated. Bond lengths are shown in monomer fragment of the nanobracelet below projections.

parameters within the monomer do not change whereas the change of energy of nanobracelet per one monomer exponentially decreases with the increase of the number of monomers both for the nanobracelets with and without hydrogen atoms at the edge of polycyclic regions. Thus approximately the same monomer structure and electronic properties can be expected for nanobracelets consisting of more than 5 monomers which are too large for DFT calculations.

Some difference between the nanobracelets with even and odd numbers of monomers is observed both for the nanobracelets with and without hydrogen atoms at the edge of polycyclic regions. Namely, the nanobracelets consisting of odd number of monomers have the lower HOMO energy, the greater HOMO-LUMO gap and the greater bond length variation in the carbon atomic chains than the nanobracelets consisting of even number of monomers. The nanobracelets with hydrogen atoms have the lower amplitude of the HOMO-LUMO gap oscillation with the number of monomers and the lower absolute values of both HOMO and LUMO energies than the nanobracelets without hydrogen atoms. Thus the nanobracelets with hydrogen atoms would easier donate electron, while the pure carbon nanobracelets would easier accept electron. There is good indirect evidence on formation of carbon nanobracelets with double chains consisting of one monomer [16]. We hope that the present study will stimulate further efforts to synthesize various carbon nanobracelets.

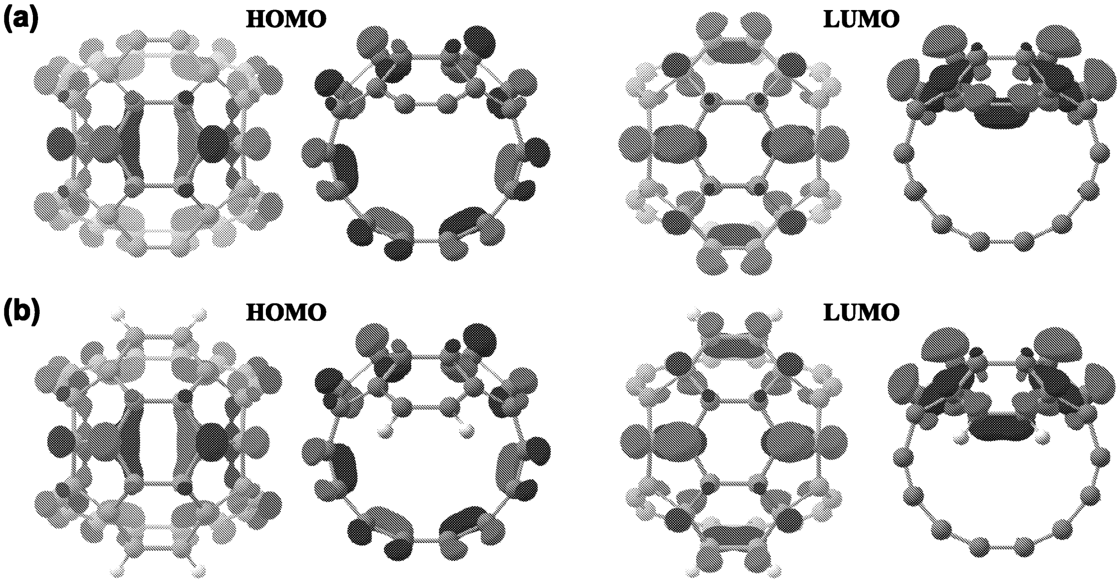

**Fig. 3.** HOMO and LUMO (highest occupied molecular orbital and lowest unoccupied molecular orbital) electron density for the smallest carbon nanobracelet consisting of one monomer without hydrogen atoms (a) and with hydrogen atoms (b).

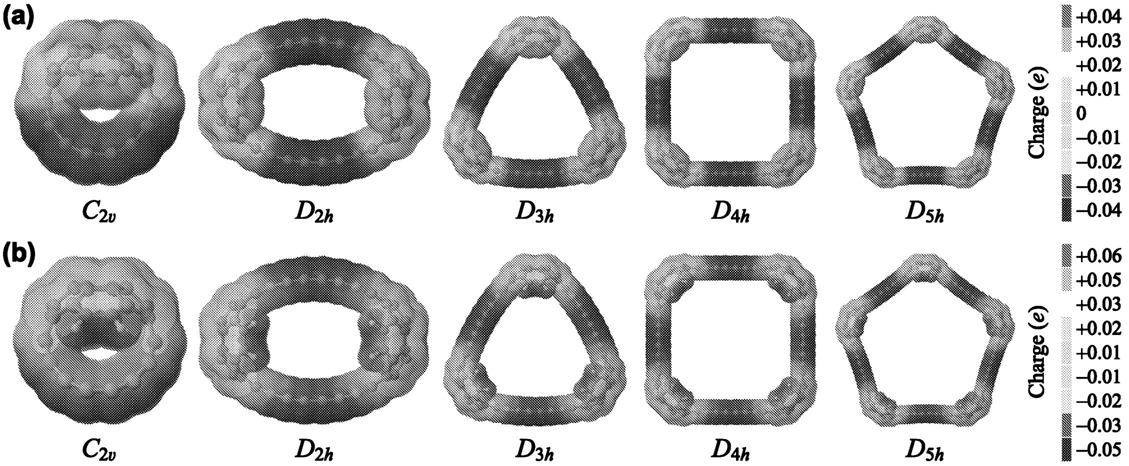

**Fig. 4.** Charge distribution in the carbon nanobracelets without hydrogen atoms (a) and with hydrogen atoms (b). Charge values are in the units of the elementary charge *e*. Corresponding point symmetry groups $C_{2v}$–$D_{5h}$ of the nanobracelets are indicated.

## CRediT authorship contribution statement

**Sergey A. Vyrko:** Investigation, Methodology, Visualization, Writing – review & editing. **Yulia G. Polynskaya:** Investigation, Writing – original draft. **Nikita A. Matsokin:** Investigation, Visualization. **Andrey M. Popov:** Conceptualization, Writing – original draft. **Andrey A. Knizhnik:** Methodology, Software. **Nikolai A. Poklonski:** Funding acquisition, Project administration, Supervision, Writing – review & editing. **Yurii E. Lozovik:** Funding acquisition, Project administration, Supervision, Writing – review & editing.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

The raw data that support the findings of this study are openly available in Mendeley Data at https://doi.org/10.17632/jx6b58kfyy, see Ref. [38].

## Acknowledgments

Y.G.P, A.M.P., and Y.E.L. acknowledge the support by the Russian Science Foundation grant No. 23-42-10010, https://rscf.ru/en/project/23-42-10010/. S.A.V. and N.A.P. acknowledge support by the Belarusian Republican Foundation for Fundamental Research (Grant No. F23RNF-049) and by the Belarusian National Research Program "Convergence-2025".

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