Abstract: In the flames during low-pressure combustion, not only a rich variety of fullerenes but also many reactive intermediates can be produced (e.g., carbene, CH$_2$) that are short-lived and cannot be stabilized directly under normal circumstances. These intermediates can be captured by fullerene carbon cages for stabilization. In this paper, three C$_{71}$H$_2$ isomers were synthesized in situ in low-pressure benzene-acetylene-oxygen diffusion flame combustion. The results, which were unambiguously characterized by single-crystal X-ray diffraction, show that the three isomers are carbene addition products of D$_{5h}$-C$_{70}$ on different sites. The relative energies and stability of different C$_{71}$H$_2$ isomers are revealed by Ultraviolet-Visible (UV-Vis) absorption spectroscopy, in combination with theoretical calculations, in this work. Both the in situ capture and theoretical study of these C$_{71}$H$_2$ isomers in low-pressure combustion will provide more information regarding carbene additions to other fullerenes or other carbon clusters at high temperatures.

Keywords: low-pressure combustion; fullerene derivatives; in situ capture; carbene addition

1. Introduction

The soot produced from the combustion of gaseous fuels at low pressure contains a rich variety of polycyclic aromatic hydrocarbon and fullerenes, including C$_{60}$, C$_{70}$, and other conventional IPR-satisfying (IPR—isolated pentagon rule) [1] fullerenes [2,3] and some special IPR-violating fullerenes [4–7]. Similar to the free-radical reactions in organic chemistry [8], electron-deficient fullerenes, such as C$_{60}$ and C$_{70}$, can act as free radical scavengers [9,10] to capture and stabilize the reactive species formed in the combustion process. The well-defined structures of fullerene derivatives provide important experimental evidence for the study of the combustion mechanism. C$_{60}$(C$_5$H$_6$) was the first C$_{60}$ derivative isolated from combustion products [11]. Our group reported a series of C$_{60}$ derivatives involving methyl-substituted cyclopentadienyl (C$_5$p$_n$) species in a low-pressure acetylene-cyclopentadiene-oxygen flame, in the form of C$_{60}$(C$_5$p$_n$(CH$_2$)$_n$) ($n = 0–4$), in which the proposed C1/C2 mechanism clearly explained the formation of curvatures in nanocarbon materials [3]. Although fullerene derivatives are prevalent, the chemical properties of C$_{70}$ derivatives in low-pressure combustion flames have rarely been discussed. C$_{70}$(C$_{14}$H$_{10}$) and C$_{70}$(C$_5$H$_6$)$_2$ [2] were isolated from the products of benzene-acetylene flame combustion, and the structures of these two C$_{70}$ derivatives were determined in combination with theoretical simulation, i.e., the adducts obtained by the Diels–Alder reaction of the C$_{14}$H$_{10}$ and C$_5$H$_6$ groups with D$_{5h}$-C$_{70}$, respectively. However, the structures of other C$_{70}$ derivatives in the flame are still unknown, mainly because the combustion products are very complex, making isolation and purification difficult.

D$_{5h}$-C$_{70}$ is the second most abundant product (after I$_h$-C$_{60}$) of the combustion products [12–17], with five unequal carbon atoms being present in its carbon cage, resulting in eight different C–C bonds (as shown in Figure 1). There are many reactive carbene...
Acetylene and oxygen were bought from Yidong Gas Co. (Xiamen, China). Toluene was used after distillation via standard procedures. All gases and other chemicals were purchased from commercial suppliers and were used as received. Benzene and toluene were bought from Sinopharm (Shanghai, China). Acetylene and oxygen were bought from Yidong Gas Co. (Xiamen, China). Toluene was used after distillation via standard procedures.

Previously, Wang et al. reported the theoretical calculations of the carbene addition products of $D_{5h}$-$C_{70}$ [25], and found that eight possible $C_{71}H_2$ isomers could be formed by the addition reactions of carbenes with the eight different C–C bonds on $C_{70}$, which are of types $a$–$a$, $a$–$b$, $b$–$c$, $c$–$c$, $d$–$d$, $d$–$e$, and $e$–$e$. Comparisons of the distance of the C–C bond at carbene insertion sites and the corresponding stabilization energies revealed that the isomers of $a$–$a$, $a$–$b$, $b$–$c$, $c$–$c$, $d$–$d$, and $e$–$e$ are opened structures of carbene addition, called homofullerenes, while the $a$–$b$, $c$–$c$, and $d$–$e$ isomers are conventional cycloaddition structures, known as methanofullerenes [26]. It has been reported that carbenes were added to the distinct sites of $C_{70}$ to form various $C_{71}H_2$ isomers, which were subsequently fully characterized [18–21]. The synthesis of $C_{71}H_2$ could be achieved by solution chemical reactions [19–21], photochemical reactions [27], the Krätschmer–Huffman method [28,29], and pyrogenic synthetic methods [25]. However, the formation of $C_{71}H_2$ through the in situ capture of carbene by $C_{70}$ during combustion has not yet been reported. In this paper, three $C_{71}H_2$ isomers ($C_{71}H_2$-I, $C_{71}H_2$-II, and $C_{71}H_2$-III) were successfully synthesized from low-pressure benzene-acetylene-oxygen diffusion flame combustion; these were definitely characterized as $c$–$c$, $a$–$b$ and $e$–$e$ isomers by mass spectrometry, UV-Vis spectrometry, and single-crystal X-ray diffraction. The relative concentrations and stability of the three isomers were verified by theoretical calculations. The capture of these three carbene derivatives of $D_{5h}$-$C_{70}$ will be helpful for carbene addition studies at high temperatures.

2. Materials and Methods

2.1. Materials

All gases and other chemicals were purchased from commercial suppliers and were used as received. Benzene and toluene were bought from Sinopharm (Shanghai, China). Acetylene and oxygen were bought from Yidong Gas Co. (Xiamen, China). Toluene was used after distillation via standard procedures.

2.2. Synthesis and Separation

Carbon soot containing $C_{71}H_2$-I, $C_{71}H_2$-II, and $C_{71}H_2$-III was produced in the low-pressure diffusion flame combustion of benzene-acetylene-oxygen, using combustion equipment designed and built by our group [6]. During the synthesis process, the pressure inside the combustion chamber was controlled at about 25 Torr and the gas flow rates of vaporized
benzene, C₂H₂, and O₂, were set to 1.0 L/min, 0.55 L/min, and 1.10 L/min, respectively. At least 500 g of soot was synthesized continuously at a yield of 3 g/h for the next separation. The synthesized carbon soot was ultrasonically extracted 3–5 times, with toluene as solvent, and was then filtered and concentrated at room temperature. The toluene extracts were separated and purified, then analyzed with a Shimadzu LC-6AD high-performance liquid chromatograph (HPLC) (Shimadzu Co., Kyoto, Japan) in which toluene was used as the mobile phase; the Cosmosil Buckyprep column (i.d. 20 × 250 mm and i.d. 10 × 250 mm) and Cosmosil 5PBB column (i.d. 10 × 250 mm) were used alternately as stationary phases. The chromatogram was monitored at 330 nm during the separation. The procedures for product isolation are detailed in Figures S1 and S2 of the Supplementary Materials, where mass spectrometry (MS) was used after each step to confirm the purity of the samples, ultimately obtaining C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III with high purity (up to 99%). The yields of C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III in carbon soot were roughly 0.035 mg, 0.18 mg, and 0.85 mg, respectively, which were considerably lower than those of C₆₀ and C₇₀ in the carbon soot (2.5 g and 1.25 g, respectively) (see Table S1).

2.3. Characterization

Mass spectrometry (MS) was performed on a Bruker HCT mass spectrometer (Bruker Co., Karlsruhe, Germany), interfaced with an atmospheric pressure chemical ionization ion source (i.e., APCI-MS) in negative ion mode. Single-crystal X-ray diffraction data were collected on an Agilent SuperNova diffractometer (Agilent Technologies Ltd., Cheadle, UK) using a Cu Kα (λ = 1.54184 Å) microfocus X-ray source. The crystal data processing was carried out through CrysAlisPro. Within Olex2 [30], the structures were solved with the SHELXT and SHELXL-2015 [31] programs (George M. Sheldrick, Georg-August Universität Göttingen, Tammannstraße 4, Göttingen 37077, Germany), using the intrinsic phasing method, and refined using the full-matrix least-squares analysis based on F². The SQUEEZE program, part of the crystallographic software PLATON package (Version: 91117, (C) 1980–2021 A.L.Spek, Utrecht University, Utrecht, The Netherlands) [32], was used to calculate the disordered area of solvent and remove its contributions from the intensity data, as needed. The UV-Vis spectra were recorded on a Shimadzu UV-2550 UV-Vis spectrophotometer (Shimadzu Co., Kyoto, Japan), with redistilled toluene as a solvent.

3. Results and Discussion

3.1. Mass Spectrometric Analysis of C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III

The molecular weights of C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III were identified by the negative ion mode of APCI-MS. The ionization temperature during the experiment was set to 250 °C. As shown in Figure S3 of the Supplementary Materials, the three isomers of C₇₁H₂ had high purity; the molecular ion peaks of C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III are all around m/z 854.0, matching well with their molecular formula (C₇₁H₂). The insets in Figure S3 demonstrate that the experimental mass spectra of the three isomers are consistent with the calculated peaks for C₇₁H₂.

The three isomers were also characterized by multi-stage mass spectrometry (MS/MS). As shown in Figure S4 of the Supplementary Materials, no fragment ion peaks were found, indicating that they have good stability under high-energy conditions.

3.2. Crystallographic Identification of C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III

The black co-crystals of 2DPC[C₇₁H₂-I], 2DPC[C₇₁H₂-II], and 2DPC[C₇₁H₂-III] were formed by slow solvent evaporation from the mixed solutions of decapryrylcorannulene (DPC) [33] and C₇₁H₂-I, C₇₁H₂-II, and C₇₁H₂-III in toluene, respectively. The structures of 2DPC[C₇₁H₂-I], 2DPC[C₇₁H₂-II], and 2DPC[C₇₁H₂-III] were unequivocally revealed by single-crystal X-ray diffraction (see Figure S5 and Table S2 of the Supplementary Materials for the crystallographic details). Interestingly, the eutectic structures of these three isomers of C₇₁H₂ with DPCs indicate that the DPCs have very high flexibility. Palm-like DPCs can not only hold C₇₁H₂-I/III in a V-shape but also combine with C₇₁H₂-II in a parallel manner.
by adjusting the interactions between DPCs and C71H2 for high-quality eutectics. All DPCs and toluene molecules are omitted from Figure 2 for clarity.

![Figure 2](image)

**Figure 2.** Ball-and-stick models of C71H2-I (c–c), C71H2-II (a–b), and C71H2-III (e–e). C71H2-I and C71H2-II are methanofullerenes, C71H2-III is a homofullerene. The carbene addition sites are highlighted in red.

It can be seen from Figure 2 that the pristine cages of C71H2-I, C71H2-II, and C71H2-III are IPR-satisfying D5h-C70. Due to the different addition sites of carbenes on the C70 cages, they are isomers of each other. The structures of C71H2-I, C71H2-II, and C71H2-III correspond to the c–c, a–b, and e–e types of the C71H2 isomers, respectively, as demonstrated in the theoretical calculations [25]. Among them, the carbene additions of c–c and a–b isomers are similar to the “2 + 1” cycloaddition reactions in organic synthesis. Both c–c and a–b isomers exhibit C2v symmetry and belong to the methanofullerenes. However, the carbene of the e–e isomer is added at the equatorial site of C70 in an opened structure, resulting in the C2v symmetric homofullerene.

3.3. UV-Vis Spectra of C71H2-I, C71H2-II, and C71H2-III

The purified C71H2-I, C71H2-II. And C71H2-III could be dissolved in common solvents, such as toluene, benzene, o-dichlorobenzene, and carbon disulfide. The solutions of C71H2-I and C71H2-II are yellowish-brown, while the solution of C71H2-III is reddish-brown, similar to that of C70. As shown in Figure 3, the three isomers of C71H2 have obvious absorption peaks in the UV-visible region. It can be seen that the UV-Vis spectra of C71H2-I (c–c) and C71H2-II (a–b) are very similar, while the UV-Vis spectrum of C71H2-III (e–e) is similar to that of D5h-C70. This phenomenon is consistent with Smith et al.’s previous proposal [20] that homofullerenes hold the π electron conjugation of the C70 skeleton to the greatest extent. In addition, the onset wavelengths of C71H2-I (c–c), C71H2-II (a–b), and C71H2-III (e–e) gradually decrease, indicating that their optical energy gaps (Eg) increase progressively.
D5h

D

a

b

e

a–b

d–e

D

S6 of the Supplementary Materials. Compared to D5h-C70, the stability of the carbene insertions slightly decreases because of the higher HOMO/LUMO energies. Of all the eight C71H2 isomers, e–e is the most stable, while d–e and c–d are the least stable. With the insertion of carbenes, the distance of the C–C bonds at the insertion sites on D5h-C70 will change, where the distance of e–e becomes 2.315 Å, while those of a–b and c–c are only 1.647 Å and 1.612 Å, respectively. The electrostatic potential surface details of the C71H2 isomers and D5h-C70 are shown in Figure S7 of the Supplementary Materials, indicating that the electrostatic potentials of the carbene fragments are more positive than those of the rest of the caged fragments.

Table 1. DFT calculation results of C71H2 isomers and D5h-C70 at the B3LYP/6-31G(d,p) level.

|        | HOMO | LUMO | H-L gap  | R_C-C (Å)      | ΔE (kcal/mol) |
|--------|------|------|----------|----------------|---------------|
| D5h-C70|      |      |          |                |               |
| e–e    | −5.92| −3.24| 2.69     | 2.315 a (1.471 b) | 0.00          |
| a–b    | −5.66| −3.10| 2.55     | 1.647 a (1.397 b) | 9.88          |
| d–d    | −5.72| −3.19| 2.52     | 2.154 a (1.434 b) | 11.62         |
| c–c    | −5.64| −3.12| 2.52     | 1.612 a (1.389 b) | 11.77         |
| a–a    | −5.78| −3.15| 2.63     | 2.183 a (1.452 b) | 12.59         |
| b–c    | −5.78| −3.14| 2.65     | 2.181 a (1.448 b) | 15.30         |
| c–d    | −5.71| −3.16| 2.55     | 2.178 a (1.449 b) | 22.81         |
| d–e    | −5.74| −3.14| 2.60     | 2.131 a (1.421 b) | 23.70         |

a The C-C bond distance of the carbene insertion sites. b The relative C-C bond distance in pristine D5h-C70.

To gain a deeper insight into the relative abundances of all possible isomers of C71H2 at high temperatures, the rigid rotor and harmonic oscillator (RRHO) approximation [34] was employed and the Gibbs energies of isomers from 0 K to 5000 K were calculated. As shown in Figure 4, the e–e isomer is the most abundant among the C71H2 isomers over the entire temperature range, from 0 to 5000 K. As the temperature rises to around 3200 K, the relative concentrations of the other seven isomers tend to change to flat, at which point the a–b and c–c isomers become the second and third stable isomers after the e–e isomer. With the temperature gradually increasing, the relative concentrations of a–a, c–c, and
d–d isomers change slightly but very closely, which corresponds to the relative energies resulting from the theoretical calculations in Table 1.

![Figure 4](image)

**Figure 4.** Relative concentrations for the C$_{71}$H$_2$ isomers, based on the RRHO approximation.

It can be seen that the capture of C$_{71}$H$_2$-I (c–c), C$_{71}$H$_2$-II (a–b), and C$_{71}$H$_2$-III (e–e) is not accidental. According to the calculation results in Table 1 and Figure 4, e–e (0.00 kcal/mol) and a–b (9.88 kcal/mol) are the first and second stable isomers with the highest concentrations at high temperatures, respectively. Although the relative energies and relative concentrations of the a–b and d–d isomers are close to each other, the isomer captured in this work is e–e. The reason for this may be that the C–C bond in $D_{3h}$-C$_{70}$ is an independent double bond (1.389 Å) at the e–e site, while the d–d site (1.434 Å) is only a small fragment of the aromatic region and carbenes prefer double bonds to the larger aromatic regions (Figure S8). Therefore, the c–c isomer may be more easily generated than the d–d isomer under identical experimental conditions. Accordingly, the stability of C$_{71}$H$_2$-I (c–c), C$_{71}$H$_2$-II (a–b), and C$_{71}$H$_2$-III (e–e) gradually increase. This was also verified by the UV-Vis spectral analysis in Figure 3, where the optical energy gaps (Eg) of C$_{71}$H$_2$-I, C$_{71}$H$_2$-II, and C$_{71}$H$_2$-III are presumed to increase gradually. Their $^1$H NMR spectra are also simulated by theoretical calculations (Figure S9 in the Supplementary Materials). The other five isomers have not been isolated under the currently available synthetic conditions, probably because of their higher energies and lower stability than the three isomers obtained in this paper.

In the combustion processes of gaseous fuels, fullerenes might be produced from the continuous growth of intermediates, such as polycyclic aromatic hydrocarbons, bowl-shaped polycyclic aromatic hydrocarbons, and small carbon radical molecules [3,35–40]. The present work not only provides explicit structural characterizations of C$_{70}$ carbene addition isomers but will also inspire further explorations into the capture of active intermediates and our understanding of the formation mechanism of fullerenes in combustion. Further investigations on the formation mechanism of fullerenes in combustion are still ongoing.

4. Conclusions

In summary, three C$_{70}$ derivatives of carbene addition, C$_{71}$H$_2$-I (c–c), C$_{71}$H$_2$-II (a–b), and C$_{71}$H$_2$-III (e–e), were successfully synthesized by low-pressure benzene-acetylene-oxygen diffusion flame combustion. The crystal structures of the three isomers have been unambiguously characterized by single-crystal X-ray diffraction. The crystallographic data show that C$_{71}$H$_2$-I and C$_{71}$H$_2$-II are methanofullerenes, while C$_{71}$H$_2$-III is a homofullerene. The band gaps and the relative stability that was estimated from the UV-Vis absorption spectra of the three isomers are in good agreement with the theoretical calculation results, indicating that their formation is not accidental. The synthesis of these three C$_{71}$H$_2$ isomers
also indicated that the reactive and short-lived carbene intermediates in the flame of low-pressure combustion could be captured and stabilized by fullerene carbon cages. In the low-pressure flame from gaseous fuels, carbene and other small carbon radical molecules play very important roles in the growth of fullerenes. The current work could inspire further exploration of the capture of reactive intermediates and insights into the mechanism of fullerene formation in combustion.

**Supplementary Materials:** The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/nano12183087/s1, Figure S1: HPLC chromatograms for the separation of C_{71}H_{2}-I and C_{71}H_{2}-II. (The shaded areas correspond to the collected components containing C_{71}H_{2}-I/II). (a), (b), (c) and (d) correspond to the HPLC separation chromatograms of C_{71}H_{2}-I and C_{71}H_{2}-II in the first, second, third and fourth stage, respectively; Figure S2: HPLC chromatograms for the separation of C_{71}H_{2}-III. (The shaded areas correspond to the collected components containing C_{71}H_{2}-III). (a), (b), (c) and (d) correspond to the HPLC separation chromatograms of C_{71}H_{2}-III in the first, second, third and fourth stage, respectively; Figure S3: APCI-MS spectra of C_{71}H_{2}-I (a), C_{71}H_{2}-II (b) and C_{71}H_{2}-III (c) in toluene. (The insets show the experimental and simulated isotopic distributions); Figure S4: MS-MS spectra of C_{71}H_{2}-I (a), C_{71}H_{2}-II (b) and C_{71}H_{2}-III (c) in toluene; Figure S5: C_{71}H_{2}-I (a), C_{71}H_{2}-II (b) and C_{71}H_{2}-III (c) molecules and two co-crystallized DPC molecules in the unit. (C gray, H cyan, N navy blue); Figure S6: The highest occupied molecular orbitals and lowest unoccupied molecular orbitals of C_{71}H_{2} isomers and D_{3h}-C_{70} at B3LYP/6-31G(d,p) level; Figure S7: The electrostatic potential surfaces of C_{71}H_{2} isomers and D_{3h}-C_{70} at B3LYP/6-31G(d,p) level; Figure S8: The optimized structure of D_{3h}-C_{70} at B3LYP/6-31G(d,p) level by G16 program; Figure S9: Theoretical simulations for ^{1}H NMR spectra of a-b (a), c-c (b) and e-e (c) at B3LYP/6-31G(d,p) level; Table S1: The yields of C_{71}H_{2}-I, C_{71}H_{2}-II and C_{71}H_{2}-III in soluble extracts at each separation stage; Table S2: Crystallographic data for C_{71}H_{2}-I, C_{71}H_{2}-II and C_{71}H_{2}-III.

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