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A Three-Dimensional Capsule-Like Carbon Nanocage as a Novel Segment Model of Capped Zigzag [12,0] Carbon Nanotubes: Synthesis, Characterization, and Complexation with C_{70}

Shengsheng Cui,[+a] Guilin Zhuang,[+b] Dapeng Lu,[a] Qiang Huang,[a] Hongxing Jia,[a] Ya Wang,[a] Shangfeng Yang,[a] Pingwu Du*[a]

Abstract: Herein we report the synthesis, photophysical, and supramolecular properties of a novel three-dimensional capsule-like hexa-*peri*-hexabenzocoronene (HBC)-containing carbon nanocage, tripodal-[2]HBC, which represents the first synthetic model of the capped zigzag [12,0] carbon nanotubes (CNTs). Tripodal-[2]HBC was achieved by rationally designed palladium-catalyzed coupling of triborylhexabenzocoronene and L-shaped cyclohexane units, followed by nickel-mediated C-Br/C-Br coupling and the subsequent aromatization of the cyclohexane moieties. The physical properties of tripodal-[2]HBC and its supramolecular host-guest interaction with C_{70} were further studied by UV-vis and fluorescence spectroscopy. Theoretical calculations reveal that the strain energy of tripodal-[2]HBC is as high as 55.2 kcal·mol^{-1}.

Carbon nanotubes (CNTs) have attracted much attention over the last few decade due to their interesting physical and electronic properties,[1] which greatly depend on their size, edge structure, and chirality.[2] So far, It is still a great challenge to achieve controlled synthesis of CNTs.[3] To mimic the segment models of CNTs, organic molecules with hoop-shaped π-conjugated systems have gained a great deal of attention due to their interesting curved structures and physical properties.[4] Cycloparaphenylenes (CPPs), the simplest structural unit of armchair carbon nanotubes, are envisioned as precursors for the bottom-up synthesis of armchair CNTs with a fixed chirality and diameter.[4a,5] In 2003, using a top-down strategy by detraction of the conjugated system of [60]fullerene, the successful synthesis of a cyclic benzenoid [10]cyclophenacene as a segment model of (5,5)-armchair SWNTs was reported.[6] Since 2008, a variety of [n]CPP nanorings (n=5-18) have been reported by using different bottom-up approaches.[7] Subsequently, the congeneric armchair variants began quickly to flourish.[8] The Müllen group reported a pre-construction strategy to insert large π-extended sidewalls into CPPs.[8a] Owing to the difficulty of directly functionalizing CPPs to create a fully π-extended CNT sidewall segment, our group developed a post-construction method to insert a nanographene unit, hexa-*peri*-hexabenzocoronene (HBC), as the large π-extended sidewalls into [18]CPP and [12]CPP backbones.[9]

Besides these armchair CNT models, several chiral carbon nanorings[10] and branched CNT segments[11] have also been reported. Despite these intense studies, however, the study of (n,0)-zigzag CNT segments as another important model compound continues to be limited and no large π-extended polyaromatic hydrocarbons (PAHs, for example, HBC unit) have been used as the capping unit to build the segment of a capped carbon nanotube. The chemical synthesis of finite models of zigzag single-walled CNTs, for example, cyclacenes, still remains a great challenge due to its highly reactive open-shell nature.[12]

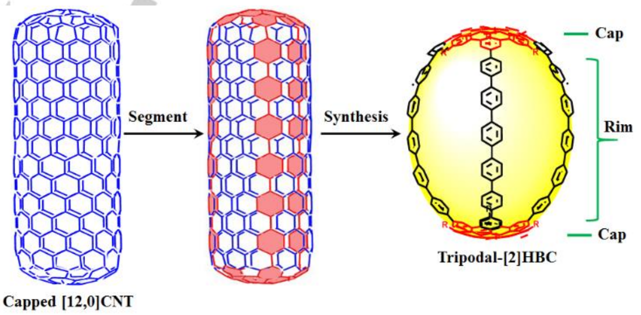

Figure 1. The design of tripodal-[2]HBC carbon nanocage as a novel finite model of capped [12,0] carbon nanotube.

Herein we report the synthesis of a novel three-dimensional capsule-like large π-conjugated molecule, tripodal-[2]HBC which represents the zigzag [12,0] CNT model with two large polycyclic aromatic hydrocarbon end caps (Figure 1). Unlike the previously reported sidewall type segments in the infinite CNT structures, this molecule is the first example of a closed CNT model with a fixed length by connecting two end caps with three olig(para-phenylene) rims symmetrically. Our synthesis involves the construction of one key building precursor, namely tripodal HBC units, and the subsequent cyclic assembly through transition metal mediated multi-fold coupling reactions. The resulting molecule was characterized by mass spectrometry (MALDI-TOF-MS) combined with nuclear magnetic resonance (NMR) spectroscopy. In addition, its photophysical and electronic properties were investigated by steady-state spectroscopy and theoretical calculations.

The HBC unit with mesityl groups is a good building block because of its high solubility in most common organic solvents, which was firstly reported by Shinokubo and co-workers.[13] Mesityl groups can be introduced at the HBC periphery by the coupling of 1,3,5-tri(3′-chlorobiphen-2-yl)benzene **3** with 2-mesitylmagnesium bromide, followed by cyclodehydrogenation with dry $FeCl_3$ (see details in supporting information). It is worth to mention that the cyclic product of HBC cannot be realized when the cyclodehydrogenation reaction is conducted after cyclization, as was shown in previous studies.[8a,8c,14] The cyclodehydrogenation step might be quite difficult due to high ring strain resulting from macrocyclization and the resulting

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complicated mixtures will make the subsequent separation and purification problematic. Therefore, it is better to conduct cyclodehydrogenation reaction prior to the macrocyclization reaction. Then the trimesityl-substituted HBC **5** was subsequently converted into the 2,8,14-triborylated trimesityl HBC **6** (Figure 2) by treatment with an excess amount of bis(pinacolato)diboron (6.0 equiv.) under iridium-catalyzed borylation conditions.[13] This convenient protocol for the introduction of boryl groups into π-rich hydrocarbons through direct C-H borylation provides a reliable method for the preparation of large quantities of *meta*-borylated trimesityl HBC, which is a key precursor for the synthesis of tripodal HBC units.

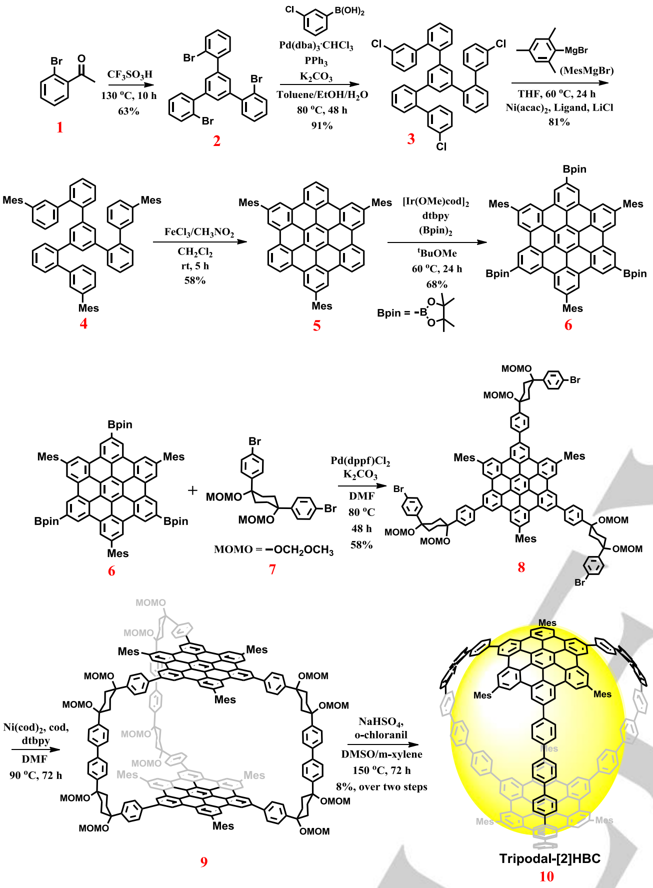

Figure 2. Synthesis procedures of *meta*-triborylated trimesityl HBC **6** precursor and tripodal-[2]HBC **10**.

The synthesis procedure of the tripodal-[2]HBC **10** is also illustrated in Figure 2. The L-shaped building block **7** was prepared by addition of 4-bromophenyllithium into cyclohexane-1,4-dione solution, followed by protection of the hydroxyls using the methoxymethyl (MOM) groups.[7c] The next step was performed to construct the tripodal HBC-containing building block **8**. The yellow solid **8** can be prepared in a high yield of 68% by the Suzuki-Miyaura cross-coupling reaction of triboryltrimesityl HBC **6** (1 equiv.) with an excess amount of **7** (12 equiv.) in the presence of Pd(dppf)Cl_2 catalyst (8.75 mol%), K_2CO_3 (12 equiv.), and anhydrous DMF at 90 °C for 48 h under nitrogen atmosphere. Next, the Ni(cod)$_2$-mediated Yamamoto coupling reaction was applied for the synthesis of **9** in the presence of **8** (1 equiv.), Ni(cod)$_2$ (6.0 equiv.), 1,5-cyclooctadiene (0.1 mL), and 4,4′-di-*tert*-butyl-2,2′-bipyridyl (6.0 equiv.) in dry DMF at 90 °C for 72 h under nitrogen atmosphere.[13,15] The good planarity and high rigidity of the HBC fragment in the backbone of the building precursor probably have a deleterious effect on the conformation for cyclization, since the yield for this step is relatively low. Subsequently, the crude product **9** obtained *via* the macrocyclization step was directly subjected to aromatization without thorough purification. The cyclohexane-1,4-diyl moieties were facilely converted to the corresponding benzene rings with $NaHSO_4 \cdot H_2O$ in mixed DMSO and *m*-xylene at 150 °C for 2 days in air. After extensive purification initially by flash column chromatography and then by preparative thin layer chromatography, the target molecule **10** was obtained in ~8 % yield over two steps as a yellow solid.

This target compound **10** was characterized by ^{1}H NMR, and MALDI-TOF mass spectrometry, and elemental analysis. Its isotopic mass peak pattern obtained in the high resolution MALDI-TOF mass spectrometry was in good agreement with the simulated values (Figure 3a, observed at m/z 3117.2997, calculated for $C_{246}H_{162}$ $[M]^+$: 3117.2944). Further characterization by ^{1}H NMR spectroscopy confirmed the successful synthesis of **10** (see SI).

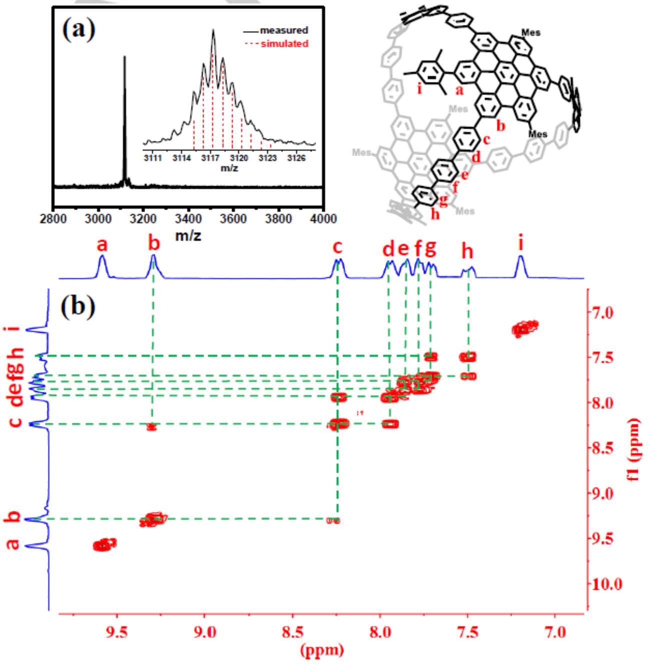

Figure 3. (a) MALDI-TOF MS and (b) Expanded 2D ^{1}H-^{1}H COSY NMR spectrum (400 MHz, CD_2Cl_2) of tripodal-[2]HBC.

The characteristic singlets at δ = 9.58 ppm and 9.29 ppm should be assigned to protons in the HBC units (a and b type protons in Figure 3b), on the basis of anisotropy effect of the HBC structure.[13,15] Another six doublets from δ = 8.23 to δ = 7.49 are rooted in the benzene rings which connect two HBC units after the acid-mediated aromatization of compound **9**. In addition, the singlet at δ = 7.19 and the singlets at δ = 2.48 ppm and δ = 2.31 ppm should be assigned to the mesitylene unit and methyl groups, respectively, verifying the highly symmetric character of the nanocage structure. To fully assign the aromatic protons in tripodal-[2]HBC **10**. 2D ^{1}H-^{1}H COSY NMR spectrum was further measured and the results are shown in Figure 3b. The singlet at δ = 9.29 exhibits a correlation relationship with proton signal at δ = 8.23, suggesting that proton at δ = 9.29 can be assigned to b site and the doublet δ = 8.23 belongs to c site. Moreover, this proton signal at δ = 8.23 is strongly correlated with the proton at δ = 7.95, confirming the latter is ascribed to d site. Based on the same analysis, all other aromatic peaks (d, e, f, g, and h protons)

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can be well assigned. As a result, ^{1}H NMR, 2D ^{1}H-^{1}H COSY NMR spectra, and the mass spectrometry confirmed the successful synthesis of tripodal-[2]HBC.

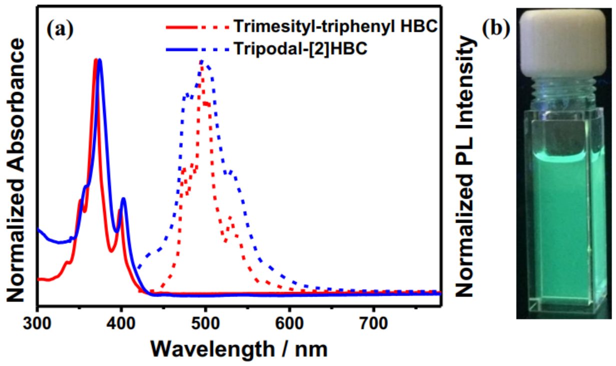

Figure 4. (a) UV-vis absorption (solid lines) and fluorescence spectra (dash lines) of tripodal-[2]HBC (blue) and trimesityl-triphenyl HBC (red) in CH_2Cl_2. (b) The photograph of the fluorescence of tripodal-[2]HBC in CH_2Cl_2 under a UV lamp (365 nm).

UV-vis absorption spectroscopy and steady-state fluorescence spectroscopy were used to investigate the photophysical properties of tripodal-[2]HBC **10** (Figure 4a, blue plot). For comparison, we synthsized trimesityl-triphenyl HBC as the reference compound (see details in supporting information), the spectra of trimesityl-triphenyl HBC was also depicted in Figure 4a (red plot). The absorption bands of **10** in dichloromethane are observed at 300-430 nm and the absorption maximum peak (λ_{max}) is observed at 374 nm with the molecular absorption coefficient (ε) of ~1 × 10^5 cm^{-1} M^{-1}. Two moderate absorption peaks were also observed with maxima at λ_{max} = 358 nm and 402 nm. It is noteworthy that the λ_{max} of the absorption bands have obvious redshift in comparison with the reference compound (trimesityl-triphenyl HBC) and those of other three-dimensional π-conjugated molecule.[11,16] This can be ascribed to a much larger π conjugation in the graphenic HBC units of the molecular structure. The fluorescence emission spectrum of **10** was studied at room temperature under an excitation of 350 nm. Multiple emission peaks were observed at 480 nm, 503 nm, and 536 nm, respectively, which also have redshift compared to the reference compound. The fluorescence quantum yield was determined to be Φ_F = 17.1% using anthracene in ethanol as the reference (Φ_F = 30%). This value is higher than that of trimesityl-triphenyl HBC (Φ_F = 14.3%), which might be due to the effect of the larger π conjugation after aromatization. Compound **10** shows intense green photoluminescence in CH_2Cl_2 solution under UV irradiation (Figure 4b).

Fluorescence decay measurements were performed using a nanosecond pulsed laser system in degassed CH_2Cl_2 solution at room temperature. The fluorescence decay of **10** follows first-order kinetics with a lifetime (τ_s) = 16.1 ns at 503 nm with single-exponential decay when excited at ~390 nm (Figure S1a). For comparison, trimesityl-triphenyl HBC shows a similar single-exponential decay with τ_s = 18.0 ns at 495 nm under the same excitation wavelength (Figure S1b). The fluorescence lifetime of **10** is longer than other three-dimensional π-conjugated molecule (τ_s = 1.4 ns for [6.6.6] carbon nanocage[11] and τ_s = 2.1 ns for ball-like π-conjugated molecule[16]). Taking the long fluorescence lifetime of HBC unit into consideration, the inserted HBC could contribute to the long fluorescence lifetime of **10**.[9b]

To further understand the physical properties of the present capsule-like carbon nanocage, we optimized the structure of tripodal-[2]HBC **10** by density functional theory (DFT) calculations at the PBE/DNP theoretical level using DMol^3 software.[17] The geometrical optimization result shows that the cage structure of tripodal-[2]HBC **10** has the cavity of *c.a.* 10.5 Å (Figure S2). Specifically, six trimethyl-benzol groups generate torsion angles averaging 64.4° with top or bottom aromatic moieties, while a torsion angle averaging 32.3° appears on the three para-linked aromatic chains. As shown in Figure 5, the frontier molecular orbital results indicate that HOMO mainly involves π-type bonding orbitals on the top and bottom HBC moieties, while LUMO mainly concentrates on π-type anti-bonding orbitals on one longitudinal aromatic chain and two caps. Furthermore, following two reported methods[7c,18] (Figure S3), the strain energy is estimated to be 55.20 kcal·mol^{-1}, compatible with the accepted value for cycloparaphenylenes.[18] Furthermore, the single-point calculations under the level of B3LYP/6-31G* reveal that the HOMO-LUMO gap of 3.19 eV (389 nm) is close to the experimentally observed longest-band of 402 nm.

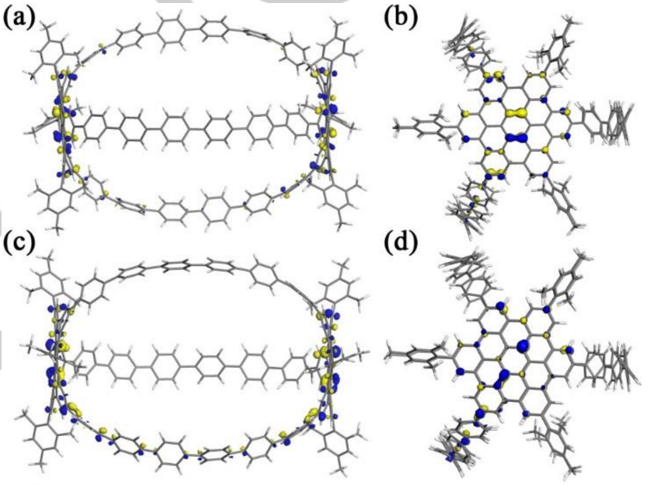

Figure 5. HOMO (a-b) and LUMO (c-d) of tripodal-[2]HBC with top view and side view.

Considering the concave cavity of tripodal-[2]HBC **10**, it could act as a supramolecular host for π-conjugated molecules with a convex surface, such as fullerenes. We next investigated the supramolecular host-guest interaction behavior between tripodal-[2]HBC and fullerene C_{60} and C_{70}. Note that no appreciable change was observed when mixing C_{60} with tripodal-[2]HBC **10**. Interestingly, the supramolecular interaction between **10** and C_{70} was clearly observed. The interaction between **10** and C_{70} was initially studied by MS spectrometry (Inset, Figure 6a). The peak observed at m/z 3958.2807 (calculated for $C_{316}H_{162}$ [C_{70}@**10**]$^+$: 3958.2777) suggests the formation of a 1:1 complex. The interaction between tripodal-[2]HBC and C_{70} was further observed by ^{1}H NMR spectroscopy when C_{70} was added to tripodal-[2]HBC in CD_2Cl_2 (Figure S4). The complexation between tripodal-[2]HBC and C_{70} was further examined by the UV-vis titration experiment and an isosbestic point located at 423 nm was observed (Figure 6a). When C_{70} was added into a solution of **10** in dichloromethane, the solution exhibited an obvious color change from yellow to light brown (Figure 6b). The resulting Job's plot of the UV-vis spectra at 374 nm in toluene showed a maximum absorption change when the ratio of tripodal-[2]HBC and C_{70} reached approximately 1:1 (Figure 6c), confirming their 1:1 complexation. Based on the UV-vis titration experiments (Figure S5), we determined the binding constant K_a of the tripodal-[2]HBC with C_{70} in toluene to be ~1.06 × 10^5 M^{-1} (Figure 6d). This K_a agrees well with the value obtained from the fluoresence titration experiment (~1.03 × 10^5 M^{-1}, Figure S6) within experimental error.

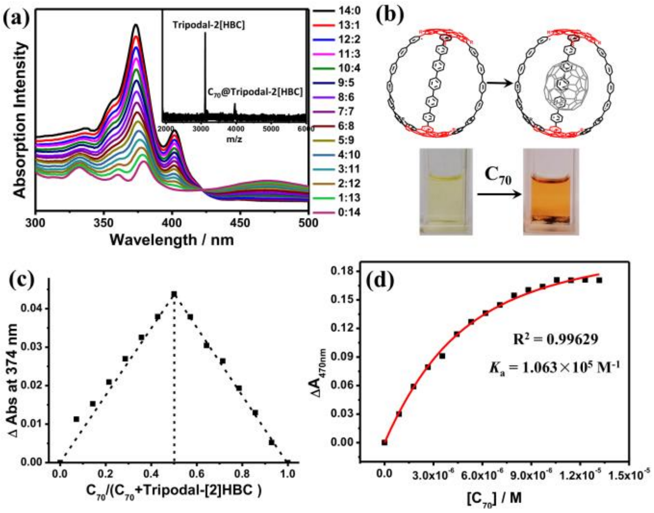

Figure 6. (a) UV-vis spectra of tripodal-[2]HBC and C_{70} at different ratios in toluene for Job's plot analysis. Insert: mass spectrometry data for the C_{70}@tripodal-[2]HBC complex. (b) Schematic drawing of the C_{70}@tripodal-[2]HBC complex. (c) Job's plot of tripodal-[2]HBC and C_{70}. (d) The plot of the absorption changes at 470 nm versus [C_{70}] in toluene for calculating the K_a. R^2 is the standard deviation.

In conclusion, we have successfully synthesized a three-dimensional, capsule-like carbon nanocage tripodal-[2]HBC **10** as a segment model compound of capped [12,0] carbon nanotubes. A straightforward method was developed for the nanocage construction using three L-shaped diphenylcyclohexane monomers to connect two HBC units. This synthesis strategy provides a rational route for the bottom-up construction of three-dimensional π-conjugated carbon nanocage. Further challenges, including designing and synthesizing large π-extended carbon nanocages more similar to capped CNT segments are the focus of ongoing work in our laboratory.

Acknowledgements

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Keywords: nanocapsule • polyaromatic hydrocarbons • π-extended • carbon nanotube segment • three-dimensional

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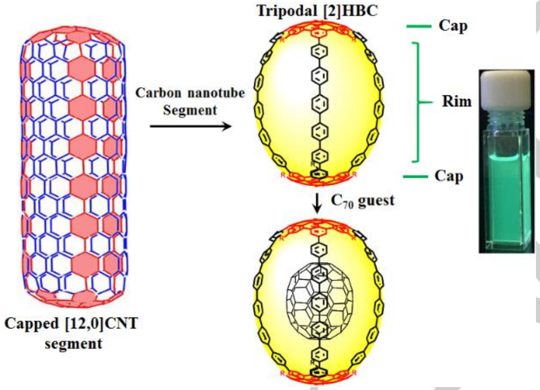
Entry for the Table of Contents

COMMUNICATION

For the first time, three-dimensional capsule-like hexa-peri-hexabenzocoronene (HBC)-containing carbon nanocage was successfully synthesized and isolated, which represents a novel synthetic model of the capped zigzag [12,0] carbon nanotubes. The photophysical properties and supramolecular interaction with C_{70} of the capsule were investigated. Theoretical calculations reveal that that its strain energy is as high as 55.2 kcal·mol^{-1}.



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