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Janusarene: A Homoditopic Molecular Host

Tao Li, Luoyi Fan, Hao Gong, Zeming Xia, Yanpeng Zhu, Nianqiang Jiang, Long Jiang, Gaofeng Liu, Yang Li, Jiaobing Wang*

Abstract: We report a kind of homoditopic molecular host, janusarene, which has two back-to-back compactly arranged nanocavities for guest complexation. The unique two-face structural feature of janusarene allows it to bind and align various guest compounds, concurrently, which include the spherical pristine fullerene C_{60} and the planar polycyclic aromatic hydrocarbons (PAHs) such as pyrene, perylene, and 9,10-dimethylanthracene. The host-guest interactions were characterized by single crystal X-ray diffraction. A pairwise encapsulation of the PAH guests by janusarene enables us to obtain PAH dimers which deliver emerging spectroscopic properties distinct from those of PAHs dissolved in solution, or in the bulk state. Moreover, a monotopic control host was synthesized and used to characterize the host-guest complexing behaviour in solution.

Advances in supramolecular chemistry depend heavily on the creations of various molecular building blocks, among which the host compounds such as crown ether, cyclodextrin, calixarene, cucurbituril, and the more recently developed pillararene (CCCCP) are prominent examples[1,2]. The popularity enjoyed by these CCCCP compounds and their derivatives stems from the well-preorganized structures, highly predictable noncovalent interactions, easy accessibility and modularity. These properties enable the CCCCP compounds to contribute significantly to different areas[3-12] of supramolecular chemistry, including but not limited to molecular recognition, self-assembly, molecular mechanics, and biomimetics. It is self-evident that even after five decades of intensive explorations, making of novel host compounds remains an important target in the field of supramolecular chemistry.

We introduce here a kind of novel molecular host, janusarene (Figure 1), which has two back-to-back compactly arranged, nanoscale binding cavities to complex with various guests, including the spherical fullerene and the planar polycyclic aromatic hydrocarbons (PAHs) such as pyrene, perylene, and 9,10-dimethylanthracene (DMA). In contrast to the contemporary widely-employed monotopic CCCCP derivatives, janusarene is homoditopic in nature[13]. This unique structure feature allows janusarene to bind and align guest molecules concurrently, by forming an alternate host-guest assembly. Moreover, to fully occupy the nanoscale binding cavities, PAH guests are encapsulated by janusarene in a pairwise manner, which leads to excimer emissions. Janusarene combines the virtues of easy synthesis, flexible modification, and well-defined architecture, these properties should benefit its further elaborations for different applications as a modular supramolecular building block in general.

The structure of janusarene mirrors that of a Janus head (Figure 1A), with two concave aromatic faces fused together in a back-to-back style and functioning as the binding cavities. We utilize the conformational preference of hexaphenylbenzene[14] (HPB, Figure 1B) platform to control both the position and orientation of the structural components. Specifically, free rotation of the peripheral phenyl rings (p-rings), along the axis of their C-C bonds to the central phenyl ring (c-ring) of HPB, is restricted due to steric hindrance[15], providing a desired conformation to construct janusarene. Six phenyl substituents are connected to each side of the HPB scaffold at the meta-position of the p-rings, thereby fencing two conical molecular spaces on the HPB "back", which can accommodate various guest compounds.

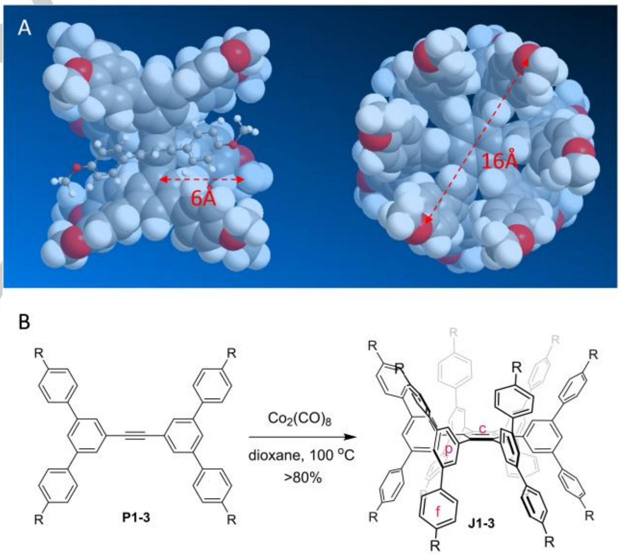

Fig. 1. (A) Space filling molecular model of **J1** optimized using molecular mechanics (left, side view; right, top view). Part of the structure is shown as ball-and-stick model to visualize the cavity. The depth (ca. 6Å, distance between the centroid of HPB and the plane of the oxygen atoms at the edge) and width (ca. 16Å, distance between the opposite oxygen atoms at the edge) of the cavity are indicated with arrows. (B) Synthesis and molecular structure of janusarene **J1-3**. **J1**, R = OMe; **J2**, R = CH_3; **J3**, R = H. Central, peripheral, and fencing phenyl rings of janusarene are labelled as c, p, and f, respectively.

The synthesis of janusarene is efficient and convenient (Figure 1B). Nineteen phenyl rings (seven of them constitute the HPB "back", the other twelve fence around the two faces) are incorporated into janusarene, in a single step, through a cobalt catalysed cyclo-trimerisation in good to excellent yield. The alkyne precursors are obtained readily using commercially available starting materials via a

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Suzuki cross-coupling. In the present study, a methoxy-substituted janusarene **J1** is used in host-guest complexations. Janusarene homologues **J2-3** are prepared to demonstrate the modularity of the synthesis. Detailed synthesis and characterization of all the related compounds are provided in the supporting materials.

Inspired by the well-established host-guest chemistry of the calixarene derivatives[16,17], we reasoned that janusarene might bind pristine fullerene via a concave-convex interaction[18-28]. This envision was further supported by a basic molecular modelling study (Figure S2), which indicated a perfect shape complementarity between C_{60} and the binding cavity of janusarene. Indeed, when a colourless solution of **J1** was added to a violet-coloured and transparent solution of C_{60} in toluene at room temperature, a dark yellow precipitate formed immediately upon mixing (Figure S3), indicating an evident noncovalent interaction.

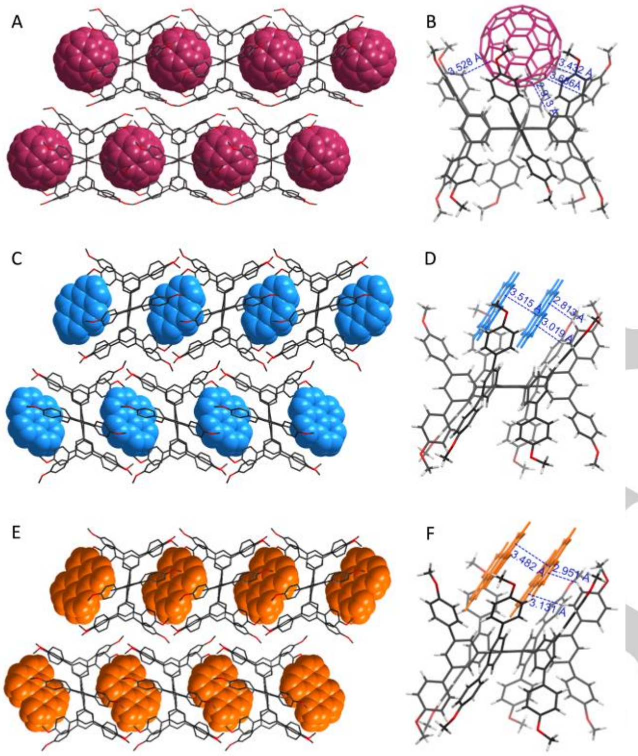

Fig. 2. Single crystal X-ray structures of the **J1**-C_{60} 1:1 (A, B, orthorhombic, Pnn2), **J1**-pyrene 1:2 (C, D, monoclinic, C2/c), and **J1**-perylene 1:2 (E, F, monoclinic, C2/c) complexes. An alternate linear assembly is observed in all cases, despite a significant change in the geometry and electronic property of the guests.

A high-quality single crystal[29] suitable for X-ray diffraction was grown in a three-layer solution (o-xylene solution of C_{60}, 0.5 mM, 4 mL, top; dioxane, 1.5 mL, middle; carbon disulfide solution of **J1**, 0.5 mM, 4 mL, bottom). Crystallographic analysis reveals a one-dimensional columnar structure (Figure 2A, B) of the **J1**-C_{60} 1:1 complex. In this structure, fullerene nestles inside the cavity formed by two adjacent janusarene molecules, manifesting a divalent supramolecular assembly[30-33]. In each column, a stacking period of 14.4 Å is observed for both C_{60} and **J1**. The columns are organized into a hexagonal packing, which is slightly disordered with an average intercolumnar distance of 15.9 Å (Figure S4). Closer examination of the crystal structure reveals intimate contact between all f-rings of **J1** and C_{60}. For each C_{60}, there are 38 neighbouring sp^2 carbon atoms from janusarene with a C-C distance < 4.0 Å (nearest C-C distance, 3.296 Å), indicating a strong concave-convex interaction. Moreover, the twelvefold C−H···π interactions between the inner protons of the HPB "back" and the π system of fullerene (C−H···π distance, 2.913 Å) should also contribute to the stabilization of the **J1**-C_{60} assembly.

Due to exceptional concave-convex complementarity, janusarene can bind and align fullerene C_{60} in a general and reliable manner. Crystallographic analysis (Figure S5) of the **J2**-C_{60} and **J3**-C_{60} 1:1 complexes demonstrates a one-dimensional divalent alternate complexation similar with the **J1**-C_{60} complex.

We find that janusarene is adaptable to bind and align non-spherical polycyclic aromatic hydrocarbons (PAHs), such as pyrene, perylene, and DMA. Despite a significant variation in the size and shape compared with fullerene, these PAH guests are encapsulated and arranged in a packing mode similar to that of the **J1**-C_{60} complex, as proved by the single crystal structures[29] (Figure 2C-F, S6). We observe an alternate one-dimensional columnar structure, in which the PAH guests locate in the cavity formed by the two neighbouring **J1** hosts. However, to fully occupy the nanoscale binding cavity, a pair of parallelly aligned PAH guests, instead of a single fullerene, are sandwiched between the janusarene hosts (**J1**: PAH = 1:2, mole ratio). The PAH dimers are slight displaced from the cofacial arrangement with short interplanar distances (ca. 3.5 Å), revealing a π-π interaction. This structural feature in crystals is maintained for all three **J1**-PAH complexes. In the crystal structure, C−H•••π interactions, van der Waals forces, and π-π stacking, cooperate to stabilize the complex (Figure 2D, F).

Comparison between the **J1**-C_{60} and **J1**-PAH crystal structures reveals that the shape of the binding cavity is adjustable to maximize the host-guest complexation through a subtle change in the dihedral angles (DA) of the p-c rings and that of the p-f rings (table S3). But, in general, the two-face, biconcave structural feature of janusarene is maintained through the unique conformation of the HPB platform, which displays an average DA^{p-c} of ca. 67° for all the crystal structures of the janusarene complexes. From this point of view, janusarene is a well-preorganized molecular host with appropriate tunability to complex with various guests such as fullerene and PAHs, as demonstrated above.

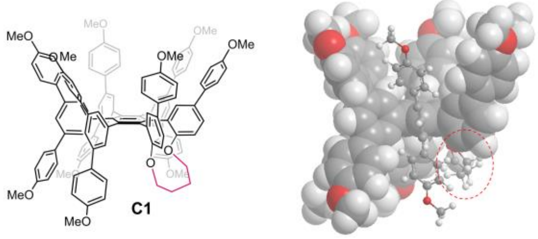

Fig. 3. Molecular structure of the control host **C1**. Replacing two f-rings of **J1**, on one side of the HPB "back", with a short aliphatic linker (circled area in the model) removes one of its binding cavity, and results in the monotopic host. Space filling molecular model of **C1** was optimized with Spartan software, MM force field.

To examine the host-guest interactions in solution, we designed and synthesized a control host **C1** with only one binding cavity (Figure 3). The monotopic nature of **C1** suggests that it may form discrete host-

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guest complex, instead of the extended assembly (for C_{60}) as observed for the homoditopic janusarene, thereby enabling us to perform the titration experiments to quantify the binding event. As shown in Figure 4A, a broad absorption band round 450 nm appears and develops when **J1** is added to a solution of C_{60} in toluene. This spectral change can be attributed to the change-transfer (CT)[34] transition from the **C1**-C_{60} complex. The solution of C_{60} changes from violet to brown in the presence of one equiv. of **C1** (Figure S2). Cyclic voltammetry measurement shows a negative shift (ca. 30 mV) of the reduction potential of C_{60} when being complexed (Figure S13), a result in accord with the expectation that **C1** has an electron-donating property, which increases the electron density of C_{60} and therefore makes it more difficult to further incorporate electrons.

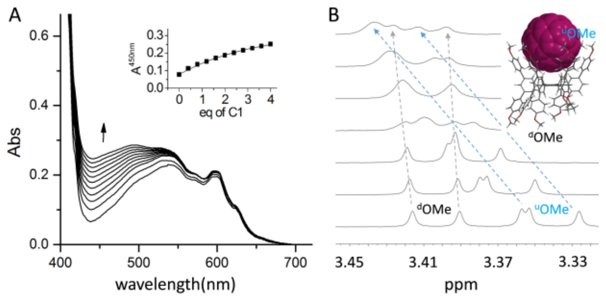

Fig.4. (A) UV-vis absorption spectral changes of fullerene C_{60} (2.0×10^{-4} M) upon addition of **C1** from 0 to 4.0 eq. Inset, titration curve with absorption at 450 nm as a function of the equiv. of **C1**. (B) Partial ^{1}H-NMR (^{8}D-toluene) spectral changes of **C1** (0.4 mM) upon addition of C_{60} from 0 to 2.4 eq. Resonance signals of the methoxy protons at the rim of the binding cavity (blue arrow, ^{u}OMe) shift to the low field when forming complex with C_{60}, in contrast to the methoxy protons away from the binding site, which show only modest spectral change (gray arrow, ^{d}OMe), inset, molecular model of the **C1**-C_{60} 1:1 complex.

^{1}H-NMR titration supports the formation of a **C1**-C_{60} complex. Protons of the methoxy groups attached at the edge of the binding cavity (^{u}OMe) experience a significant down-field shift (> 0.05 ppm) in the presence of fullerene (Figure 4B, blue arrow). Decreased electron density of the anisole-f-ring upon complex formation is expected to be responsible for the spectral changes. Job plot analysis indicates a 1:1 binding stoichiometry (Figure S9-10). An association constant of 1020 M^{-1} is derived from the titration curve (Figure S11-12). In solution, **C1** does not form the sandwich complex as observed for **J1** in the solid state (Figure 2A). This discrepancy in the binding mode, as observed for other reported fullerene complexes[22,28], may be caused by the crystal packing force. Currently, it is yet to be known whether the complexations in the two binding cavities of one janusarene are coupled to any extent.

In contrast to the spherical fullerene, titrations of **J1** or **C1** with the PAH guests in various solvent conditions such as toluene, dichloromethane (DCM), tetrahydrofuran, and mixed DCM/methanol (1:1, v/v) indicate the absence of evident host-guest interactions. This result suggests that formation of the **J1**-PAH complex occurs in and is driven by the crystalizing process. It is noteworthy that the lack of strong noncovalent interactions between janusarene and PAHs in common organic solvents does not imply that janusarene has a limited potential as a host in general, because when the solvophobic interactions are brought to bear, significantly enhanced noncovalent binding would be expected[35-37]. For instance, hydrophobic interaction is a major driving force applied by the conventional macrocycle hosts to encapsulate different guests in an aqueous environment. Primary result indicates that water soluble janusarene can associate hydrophobic guests in water with strong binding interactions, which we will report soon in a separate paper.

In the solid state, the homoditopic two-face nature of janusarene is essential to produce the **J1**-PAH complexes with a 1:2 stoichiometry (Figure 2). When the monotopic control host **C1** was used to crystalize with perylene by slow evaporation in a mixed DCM/methanol solution, a single crystal of the perylene-**C1** 1:1 complex was obtained with only one perylene residing in the binding cavity (Figure S7).

At last, we show that pairwise encapsulation of the PAHs guests by janusarene brings about emergent fluorescent properties which are absent for either free PAHs in solution, or their bulk aggregates. It is well-known that the relative orientation of chromophores plays a crucial role in determining the optical and electronic behaviour. In this context, dimers of a variety of chromophores become attractive model research targets, which may provide fundamental understanding of the basic photophysical processes and attractive spectroscopic properties possibly useful for molecular sensors, switches, light-emitting materials[38-48]. However, generation of such dimers of chromophore is neither straightforward nor general using either covalent or noncovalent approaches, a challenge well-addressed by janusarene as shown above.

We observe the excimer emissions of the PAH dimers for all three **J1**-PAH complexes at room temperature. Compared with the solution state, emission of the 0-0 band red-shifts ca. 93, 85, and 84 nm for pyrene, perylene, and DMA, respectively. These emissions are also distinct from that of the bulk PAHs, due to different orientation of the chromophore[49-52]. For instance, **J1**-perylene complex emits light at 527 nm, which can be attributed to the Y-type[53-56] excimer, and displays a blue-shift of 52 nm from that of the bulk-state at 579 nm.

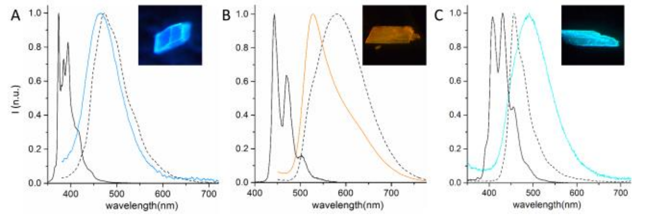

Fig.5. Normalized fluorescence spectra of pyrene (A, $\lambda^{ex.} = 310$ nm), perylene (B, $\lambda^{ex.} = 365$ nm), and DMA (C, $\lambda^{ex.} = 310$ nm) in solution (1.0×10^{-5}M, DCM, black solid line), bulk (black dash line), and encapsulated dimer (colored line, complex with **J1**) state at room temperature. Inset, vitalized emission from the crystal of the complex.

In conclusion, we present a kind of readily accessible, homoditopic molecular host, janusarene, which has back-to-back compactly arranged, nanoscale binding cavities. Taking advantage of this unique structural feature, janusarene has the ability to bind and align a variety of guest compounds, different in shape and size, including the spherical fullerene and planar PAHs. We anticipate that janusarene may find broad applications in fields such as host-guest chemistry, molecular assembly, biomimetics, and crystal engineering, which currently rely heavily on the conventional CCCCP hosts.

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Conflict of interest

The authors declare no conflict of interest.

Keywords: Janusarene • Host • Assembly • Fullerene • Excimer

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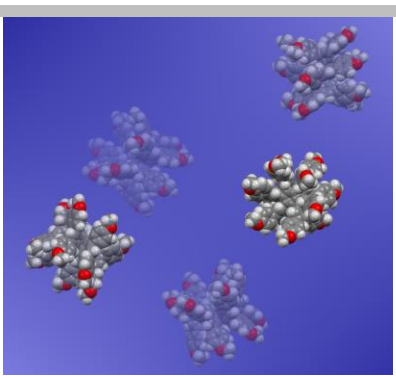

Two-face host: A kind of novel back-to-back arranged homoditopic host compound, janusarene, is presented. The unique two-face structural feature of janusarene allows it to bind and align guest compounds, varying in size and shape, such as the spherical pristine fullerene and the planar polycyclic aromatic hydrocarbons.