

Nano-Saturn with an ellipsoidal body: Anthracene macrocyclic RINGC70complex

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A macrocyclic compound consisting of six anthracene units formed a Saturn-shaped complex with fullerene C70 as the ellipsoidal guest. The association constant of the host-guest complex was determined by the NMR titration method to be $4.6 \times 10^3 \text{ L mol}^{-1}$, twice than observed for the C60 counterpart. X-ray analysis revealed that the guest molecule was included in the center of the cavity in nearly standing orientation, whereas DFT calculations predicted the complexation in various orientations. In any complex structure, CH π interactions play an important role in forming the ringbody supramolecular system. The intraannular hydrogen atoms in the ring moiety were deshielded upon complexation, and this phenomenon is discussed on the basis of the NMR shielding of C70 and the calculated structures. In spite of the different relative orientations of C70, the host-guest formation strength remains similar exposing the great versatility of the host capabilities against non-spherical fullerenes. © 2019 The Chemical Society of Japan.

Anthracene

Macrocyclic

Supramolecular system

Atoms

Energy dispersive X ray analysis

Fullerenes

Planets

Supramolecular chemistry

Titration

X ray diffraction analysis

Association constant

Complex structure

Host guest complexes

Macrocycles

Macrocyclic compounds

Pi interactions

Relative orientation

Supramolecular systems

Anthracene