



Macrocyclic Hosts for Fullerenes: Extreme Changes in Binding Abilities with Small Structural Variations

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Résumé en anglais

Exploiting the shape and electronic complementarity of C_{60} and C_{70} with π -extended derivatives of tetrathiafulvalene (exTTF), we have very recently reported a macrocyclic receptor featuring two exTTF recognizing units which forms 1:1 complexes with C_{60} with $\log K_a = 6.5 \pm 0.5$ in chlorobenzene at 298 K. This represents one of the highest binding constants toward C_{60} reported to date and a world-record for all-organic receptors. Here, we describe our efforts to fine-tune our macrocyclic bis-exTTF hosts to bind C_{60} and/or C_{70} , through structural variations. On the basis of preliminary molecular modeling, we have explored p-xylene, m-xylene, and 2,6-dimethylnaphthalene as aromatic spacers between the two exTTF fragments and three alkene-terminated chains of different length to achieve macrocycles of different size through ring closing metathesis. Owing to the structural simplicity of our design, all nine receptors could be accessed in a synthetically straightforward manner. A thorough investigation of the binding abilities of these nine receptors toward C_{60} and C_{70} has been carried out by means of UV-vis titrations. We have found that relatively small variations in the structure of the host lead to very significant changes in affinity toward the fullerene, and in some cases even in the stoichiometry of the associates. Our results highlight the peculiarities of fullerenes as guests in molecular recognition. The extreme stability of these associates in solution and the unique combination of electronic and geometrical reciprocity of exTTF and fullerenes are the main features of this new family of macrocyclic hosts for fullerenes.

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Liens

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