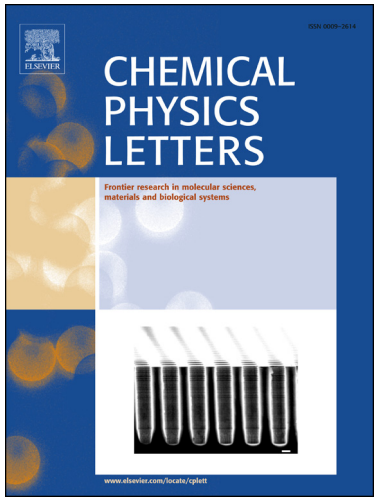

Design and characterization of two strong fullerene receptors based on ball-socket interactions

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Design and characterization of two strong fullerene receptors based on ball-socket interactions.

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Abstract

Herein, we studied the interaction between the fullerenes C_{60} and C_{70} with pentaindenocorannulene (P), chrysaorole (C) and two new buckycatchers. The P and C bowls interact with the fullerenes with an interaction-energy (IE) that is twice the value determined for corannulene. The new receptors designed include a cyclooctatetraene core which has two P or C pincers attached. Notwithstanding the fact that the proposed hosts prefer stacked conformations at equilibrium, the IE determined are extremely large and close to the ones computed for the dimeric metalloporphyrins. It is our hope that this work stimulates the synthesis of these receptors.

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1. Introduction

There is current interest in the preparation of receptors for fullerenes. In some cases, ball socket interactions [1] are the driving forces to achieve the formation of supramolecular complexes whereas in others, metalloporphyrins are employed to trap fullerenes [2-6]. Pioneering investigations by Scott and coworkers [7-8] showed that multiarmed polyarenes may be used to prepare hosts for fullerenes. However, it was not until 2007 when Sygula et al. [7] synthesized the $C_{60}H_{28}$ buckycatcher [7-16]. The receptor employs the cyclooctatetraene core and has two corannulene pincers attached. Although cyclooctatetraene is difficult to prepare, several reports have showed that it can be functionalized [17-20]. After this receptor was prepared, a plethora of new hosts have been proposed [21-298]. Without attempting to review all of them here, the following may be highlighted: pertatertbutylcorannulene [21], the contorted hexabenzocoronenes [22-23], tetrabenzoquadranulene [24], azacalix[3]-pyridine[3]pyrimidine [25], the exTTF receptors prepared by Martin and