

Binding studies of tetrathiafulvalene-calix[4]pyrroles with electron-deficient guests

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Mots-clés	Calix[4]pyrroles [13], fullerenes [14], Molecular switches [15], supramolecular chemistry [16], tétrathiafulvalènes [17] The neutral meso-octamethylporphyrinogen derivative, tetraTTF-calix[4]pyrrole 1 (TTF=tetrathiafulvalene), acts as a multi-faceted receptor in that it interacts with an assortment of different guests in different ways. The conformation of receptor 1 can be reversibly switched between the 1,3-alternate conformation (i.e., 1, Fig. 1) and the cone conformation (i.e., 1·Cl-, Fig. 2) by the repetitive addition of chloride and sodium ions. In this paper, the results of detailed and systematic complexation studies involving both 1 and its chloride-bound complex, 1·Cl-, with a variety of guests are described. Receptor 1 binds quasi-planar nitroaromatic guests in its 1,3-alternate conformation, while release of these guests takes place upon addition of chloride anions. On the other hand, spherical fullerene guests are strongly bound by 1·Cl-. Finally, it was found that a bidentate guest, consisting of a quasi-planar 2,5,7-trinitro-9-dicyanomethylenefluorene moiety tethered to a spherical C ₆₀ fullerene, could be recognized by receptor 1 in either its 1,3-alternate or its chloride-bound cone conformation, albeit through very different binding modes.
Résumé en anglais	<p>The neutral meso-octamethylporphyrinogen derivative, tetraTTF-calix[4]pyrrole 1 (TTF=tetrathiafulvalene), acts as a multi-faceted receptor in that it interacts with an assortment of different guests in different ways. The conformation of receptor 1 can be reversibly switched between the 1,3-alternate conformation (i.e., 1, Fig. 1) and the cone conformation (i.e., 1·Cl-, Fig. 2) by the repetitive addition of chloride and sodium ions. In this paper, the results of detailed and systematic complexation studies involving both 1 and its chloride-bound complex, 1·Cl-, with a variety of guests are described. Receptor 1 binds quasi-planar nitroaromatic guests in its 1,3-alternate conformation, while release of these guests takes place upon addition of chloride anions. On the other hand, spherical fullerene guests are strongly bound by 1·Cl-. Finally, it was found that a bidentate guest, consisting of a quasi-planar 2,5,7-trinitro-9-dicyanomethylenefluorene moiety tethered to a spherical C₆₀ fullerene, could be recognized by receptor 1 in either its 1,3-alternate or its chloride-bound cone conformation, albeit through very different binding modes.</p>
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