Poster

Conformational diversity of tetra-O-ethyl-*p-tert*-butylcalix[4]arene and its molecular dynamics in the single-crystal unity

R. Maria Losus[1], M. P. Krzemiński[1], L. Dobrzańska[1]

[1]*Nicolaus Copernicus University in Toruń, Faculty of Chemistry, 87-100 Toruń, Poland*
renny@doktorant.umk.pl

Ongoing research in the area of supramolecular chemistry over more than five decades has demonstrated huge structural versatility and various applications of organic macrocycles [1]. Calixarenes are one of the most extensively studied macrocycles, both in solution and in the solid state, as a result of their straightforward synthesis, well-defined and adaptable cavities, high guest binding abilities, and structural flexibility [2]. It is broadly known that calix[4]arenes can adopt four distinct conformations: *cone, partial cone, 1,2-alternate,* and *1,3-alternate*. In many cases (depending on the substituents introduced), they can switch between these conformations in solution (or the solid state). Furthermore, depending on the substituents, different conditions can be needed to initiate such interconversions. For example, in the case of tetra-ethyl-substituted calixarene, elevated temperatures are required for such conformational changes. Moreover, substitution with propyl or bulkier groups can inhibit these conformational changes altogether [3, 4].

Herein, we would like to present the results of the solid-state characterization of tetra-O-ethyl- *p-tert*-butylcalix[4]arene (CA4-Et). Three conformers of this molecule have been isolated, i.e. *cone, partial cone*, and *1,2-alternate*. Crystals of CA4-Et adopting these conformations were obtained through slow evaporation, each from a different solvent. Notably, crystals adopting the *1,2-alternate* conformation undergo a single-crystal-to-single-crystal transformation, accompanied by molecular rearrangements upon loss of solvent. The structural characteristics of the obtained conformers and an analysis of the changes taking place in the crystal during the SC-SC transformation will be discussed in detail.

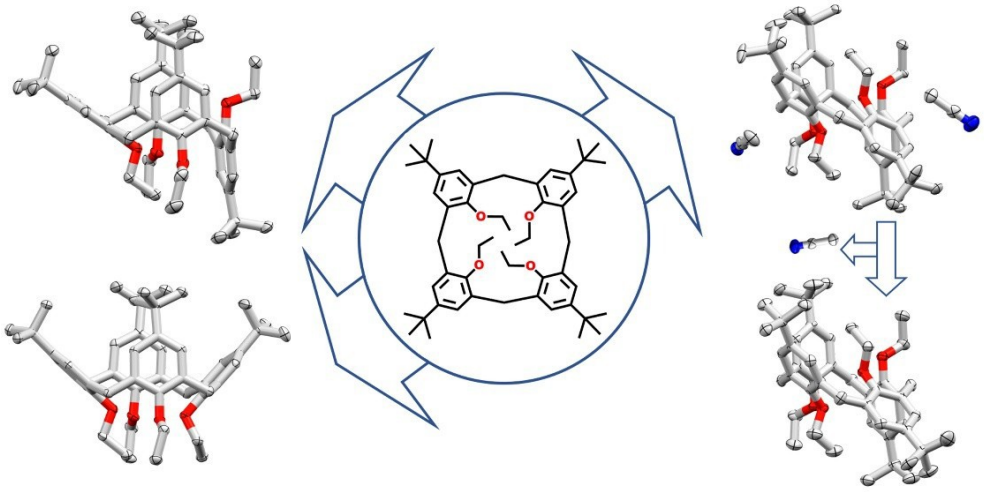

Figure 1. Schematic representation of tetra-O-ethyl-*p-tert*-butylcalix[4]arene (in the centre); crystal structures of CA4-Et adopting different conformations: *partial cone* (top left), *cone* (bottom left), *1,2-alternate* (top right) and crystal structure obtained after solvent removal (bottom right). Hydrogen atoms and disorder have been omitted for clarity.

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