

# SYNTHESIS AND PROPERTIES OF OXA[4]CALIXARENE

Anna Peterson<sup>1,2</sup>, Sandra Kaabel<sup>2</sup>, Riina Aav<sup>2</sup>, Jasper Adamson<sup>1</sup>

<sup>1</sup>Chemical Physics Laboratory, National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia

<sup>2</sup>Institute of Chemistry and Biotechnology, Tallinn University of Technology, Akadeemia tee 15, 12618 Tallinn, Estonia

e-mail of presenting author: anna.peterson@kbfi.ee

In supramolecular chemistry, calixarenes form a class of macrocyclic host molecules that have found use in a wide range of applications, such as catalysts [1], drug candidates [2] and other functional materials [3]. Specific „host-guest“ interactions are possible due to calixarene cone-like shape, macrocycles' readily functionalizable structure and multiple guest binding sites. These properties have led to extensive synthesis and design of calixarene derivatives. Heterocalixarene subfamily has evolved from this pursuit. This project focuses on oxacalixarenes, where phenol units

are connected with each other not by methylene bridges but with oxygen atoms. The different chemical and physical properties of oxacalixarenes

pave the way for finding new specifically binding guests that

can add new functionality to these type of macrocycles. In this work, unsubstituted oxa[4]calixarene was prepared based on previously reported synthesis [4]. Oxa[4]calixarene was separated and isolated from a mixture of differently-sized homologues with 40% yield. <sup>1</sup>H-NMR study confirms the structure of oxa[4]calixarene (Fig.1a) and SCXRD analysis reveals the 4-membered macrocycle to be in fixed 1,3-alternate conformation (Fig.1b). Variable temperature <sup>1</sup>H-NMR and <sup>13</sup>C-NMR study shows the conformational energy barrier to be low in solution state. Additionally, complexation properties of these macrocycles in solid phase were investigated.

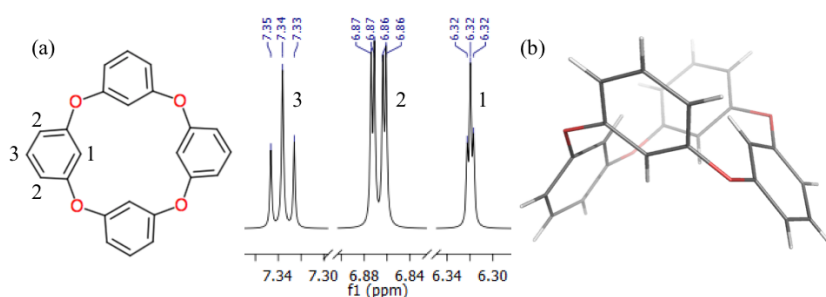


Fig. 1 (a) <sup>1</sup>H-NMR and (b) SCXRD structure of oxa[4]calixarene.

## References

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