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Poster Presentation

N-(2-acetoxyethyl)carbamoylmethoxy tert-butylthiacalix[4]arene – conformational studies

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Calixarenes are a group of the macrocyclic compounds which are widely studied due to their capability to form inclusion compounds with wide range of organic molecules. Calixarenes are known to adopt four basic conformations named cone, partial cone, 1,2-alternate and 1,3-alternate. Unsubstituted calixarenes and their derivatives with apparently small substituents at the upper and lower rim are flexible and the interexchange between the different conformations may occur. Synthesis of calixarene derivatives with bulky and/or long-chain substituents is a way to prevent conformational changes and isolate their conformationally pure isomers. Then, the inclusion properties of different conformers can be studied. In the present work X-ray structures of tert-butylthiacalix[4]arene with four N-(2-acetoxyethyl)carbamoylmethoxy

substituents at the lower rim in cone, partial cone and 1.3 alternate conformations are presented.



Keywords: thiacalixarene, conformations, co-crystals