

## Mechanism of formation of nanocavitands of cucurbit[n]uriles family. Quantum-chemical modelling.

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### Abstract

On the basis of density functional method of the version PBE quantum-chemical study of the mechanism of cucurbit[n]uriles CB[n] formation has been carried out. Reasoning from the analyses of thermodynamic characteristics of separate stages of CB[n] formation a conclusion has been made that water molecules related to oligomers, formed in the process of synthesis, exert influence mainly on the formation of CB[6], as compared to the other nanocavitands of the family CB[n].