

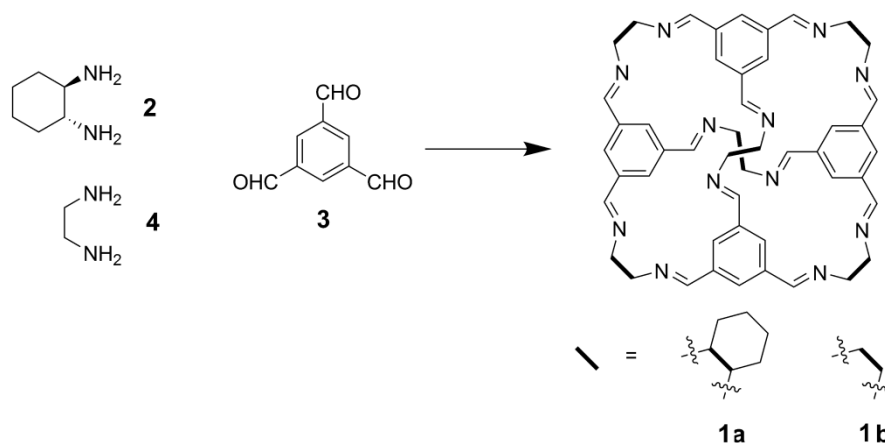
Factors affecting self-assembly of a covalent organic cage

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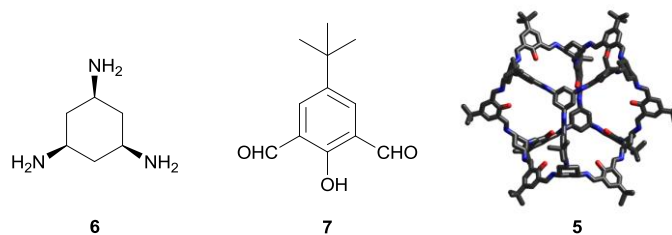
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Syntheses of highly symmetrical large size covalent organic cages raised a question what is a driving force of their formation. We have reported spontaneous formation of cage molecule (**1**) in reaction of (*R,R*)-1,2 –diaminocyclohexane (**2**) and 1,3,5-triformylbenzene (**3**) in quantitative yield.¹ Although this reaction was template-free no other products were detected by NMR of the crude material. A rare *T* symmetry structure of **1a** was confirmed by X-ray analysis.^{2,3} Similar cage was synthesized in 94% yield using conformationally labile 1,2-diaminoethane (**4**).⁴



Recently we have synthesized of an exceptionally large cage molecule (**5**) from *cis,cis*-1,3,5-triaminocyclohexane (**6**) and 4-*tert*-butyl-2,6-diformylphenol (**7**) in quantitative yield.⁴ The main factors which seems to leads to the synthesis of those molecules as the only one product seems to be stereochemical factors and entropy of symmetry.



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