Structure and Conformational Features of α-Cycloaltrin: a Cyclooligosaccharide with Alternating $^4C_1$ / $^1C_4$ Pyranoid Chairs

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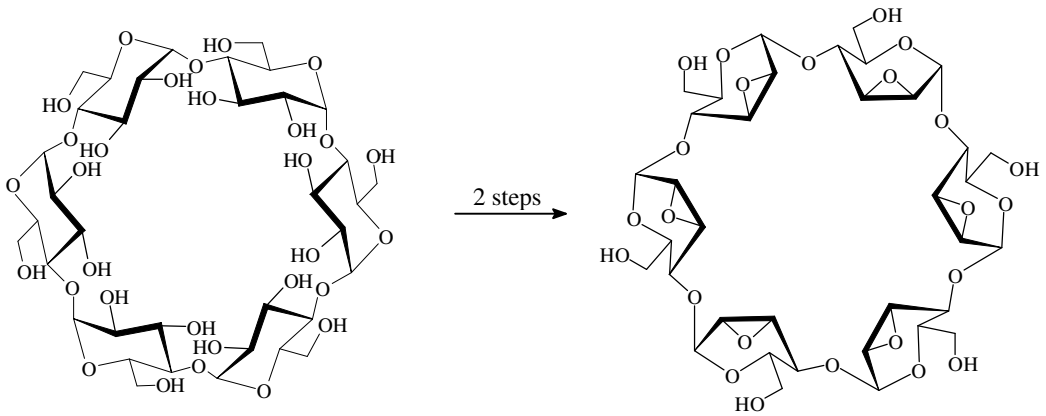
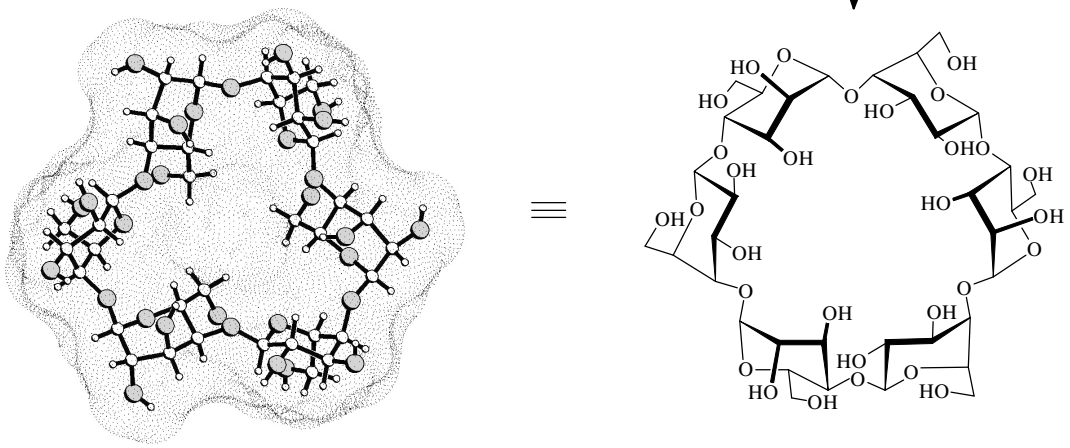
The structural characteristics of α-cycloaltrin (**3**), readily available from α-cyclodextrin (**1**) by a straightforward four-step protocol[1] with 2,3-anhydro-α-cyclomannin (**2**) as the key intermediate, has been unravelled using X-ray techniques, 800 MHz spectra (D_2O at 30 and 4°C) and molecular modeling (MD in water). In the solid state, the altropyranoid rings adopt nearly perfect $^4C_1$ and $^1C_4$ chairs in an alternating sequence, entailing the macrocycle to be devoid of a throughgoing cavity. From HTA calculations i.e. toward vacuum boundary conditions, the all-skew (twist-boat) $^0S_2$ geometry emerges as the global energy minimum structure. In water, the altropyranoid rings in **3** adopt various conformations within the $^1C_4 \rightleftharpoons {}^3H_2 \rightleftharpoons {}^0S_2$ range.



1 **2**



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[1] Y. Nogami, K. Fujita, K. Ohta, K. Nasu, H. Shimada, C. Shinohara, and T. Koga, (J. Szejtli, L. Szente, Eds.), *Proceedings 8th Internat. Symp. on Cyclodextrins*, Kluwer Acad. Publ., Dordrecht, **1996**, pp. 99-102.