α-CYCLOALTRIN: CONFORMATION AND PROPERTIES IN AQUEOUS SOLUTION

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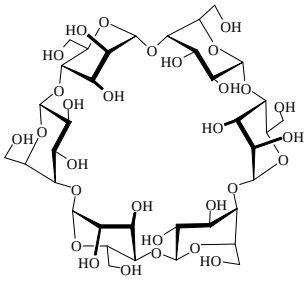
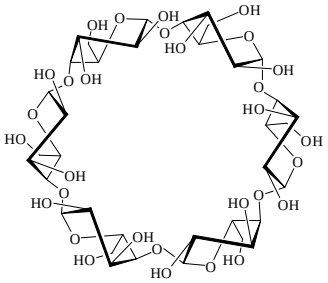
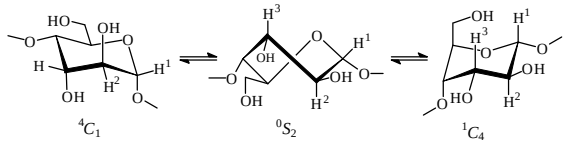
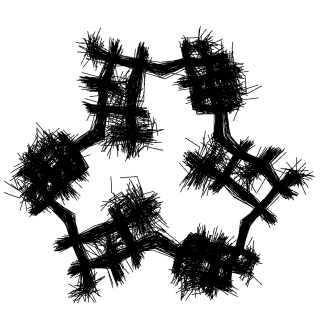
α-Cycloaltrin, readily available from α-cyclodextrin via a straightforward four-step protocol[1], adopts in the solid state[2] a C_3 symmetrical conformation with nearly perfect $^4C_1$ and $^1C_4$ chairs in an alternating sequence, but lacks a "through-going" cavity.

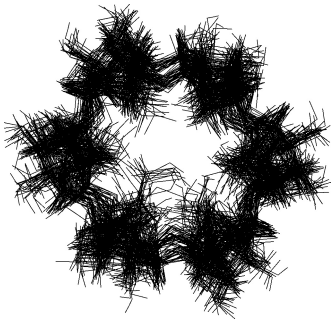






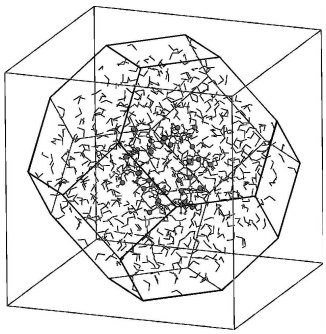
^{1}H and ^{13}C NMR experiments of α-cycloaltrin show a complex conformational equilibrium $^4C_1 \leftrightharpoons {}^0S_2 \leftrightharpoons {}^1C_4$ for each of the altrose units.





α-cycloaltrin

$^4C_1$ / $^1C_4$ conformation *all*- $^0S_2$ conformation



MD simulation box incl. 606 water molecules

Molecular dynamics (MD) simulations and temperature-dependent 800 MHz ^{1}H and ^{13}C NMR spectra (D_2O at 30 and 4°C) point toward a fast dynamic equilibrium with preferred altrose conformations in the $^1C_4 \leftrightharpoons {}^0S_2$ range. Low-temperature broadening of the C-4 and C-5 NMR signals indicate multiple conformations of α-CA in solution which are likely to ellaborate central cavities similar to those formed by cyclodextrins.

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[1] Y. Nogami, K. Fujita, K. Ohta, K. Nasu, H. Shimada, C. Shinohara, and T. Koga, *J. Incl. Phenom. Mol. Recogn. Chem.* **1996**, *25*, 57-60.

[2] Y. Nogami, K. Nasu, T. Koga, K. Ohta, K. Fujita, S. Immel, H. J. Lindner, G. E. Schmitt, and F. W. Lichtenthaler, *Angew. Chem.* **1997**, *109*, 1987-1991; *Angew. Chem. Int. Ed. Engl.* **1997**, *35*, 1899-1902.