

X-Ray Structure of a Mixed Spiroketal-Xylylene Macrocyclic Receptor

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Difructose Dianhydrides (DFAs) are a family of up to 14 diastereomeric spiroketal disaccharides formed during thermal or acidic treatment of D-fructose-containing food materials, being the major constituents of caramel [1]. Among them, the C_2 -symmetric bis-spiro di- β -D-fructopyranose isomer has been shown to exhibit strong metal cation complexing properties [2]. This unique behaviour makes it particularly attractive as building block for the construction of macrocyclic receptors. We have now prepared the first representative of this class of compounds by connecting two DFA motifs by two semirigid *p*-xylylene segments. Although the molecule conserves C_2 -symmetry in solution, as seen by NMR, the X-ray structure (data collected at the Daresbury Synchrotron) reveals desymmetrisation in the solid state. The existence of an edge-to-face interaction between the two aromatic rings is probably responsible for this situation. Interestingly, the oxygen atoms involved in cation complexing in the parent spirodisaccharide are inside directed in the macrocycle, therefore showing high promise as ion-encapsulating receptor.

[1] Rubio E., García-Moreno M.-I., Balbuena P., Ortiz Mellet C., García Fernández J. M., *Org. Lett.*, 2005, **7**, 729-731. [2] Angyal S. J., Craig D. C., Defaye J., Gabelle A., *Can. J. Chem.*, 1990, **68**, 1140-1144.

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