

Spectroscopic study of the interactions of alkali fluorides with D-xylose

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Abstract

The interactions of alkali fluorides with D-xylose have been studied by X-ray diffraction (XRD), infrared spectroscopy (IR), nuclear magnetic resonance (NMR, ^1H and ^{13}C) and atomic absorption spectrophotometry. KF and CsF form complexes with D-xylose in a 1:1 molar ratio. These complexes can be obtained by solid state milling the reactants in an agate mortar or from methanolic solutions of the sugar and the salt. LiF and NaF do not form complex with D-xylose. IR and XRD prove the identical nature of the complexes obtained by milling and from solution. IR spectra indicate strong perturbation of the OH stretching vibrations with considerable shifts to lower frequencies, which must be caused by strong hydrogen bond formation to the fluorine anion. The perturbations of C–O bond are weak, indicating that cation binding to the oxygen atoms is not the main interaction responsible for the complex formation. ^1H NMR spectra of the D-xylose–KF complex dissolved in deuterium oxide is equal to that of pure D-xylose, indicating the destruction of the complex in solution. The complex is stable in DMSO, and ^{13}C spectra of the complex in DMSO- d_6 and in solid state (CPMAS) spectra are in accordance with the observed interactions in the IR spectra. As far as we know, this is the first report of a sugar–halide salt complex in which the anion instead of the cation provides the binding forces. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The interaction of metallic cations with carbohydrates is a subject of growing interest due to the importance of these complexes in chemistry and biology. The field is well covered by extensive reviews appearing over the last 30 years [1–8]. The discovery of the interactions of boric acid and

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