X-ray structure of the dipotassium salt of D-mannose 1-phosphate 3.25 hydrate.

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2005

Czasopismo

Carbohydrate Research

Numer woluminu

340

Strony

2422-2427

DOI

10.1016/j.carres.2005.06.025

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The first crystal structure of mannose 1-phosphate is described. The dipotassium hydrate salt crystallizes in the P2(1)2(1)2 space group. There are two independent dianions (I and II) in the asymmetric unit, which are alpha anomers adopting the 4C(1) chair conformation. The main difference between the two mannose 1-phosphate dianions is the orientation of the phosphate group with relation to the pyranosyl ring. In I, one of the phosphate oxygen atoms is antiperiplanar positions with respect to carbon atom C-1, whereas the two others are situated synclinally. The corresponding orientations of the terminal phosphate oxygen atoms in II are synperiplanar and anticlinal. The potassium cations are six- and seven-coordinate, mainly with O atoms of hydroxyl groups and water molecules. There are potassium channels extending along the c-axis. In the packing arrangement, water molecules and mannose phosphate groups also define two different types of layers parallel to a-axis. Within water channels there are extensive hydrogen-bonding networks.

Słowa kluczowe

X-ray crystal structure, d-Mannose 1-phosphate, Sugar phosphates

Adres publiczny

http://dx.doi.org/10.1016/j.carres.2005.06.025

Strona internetowa wydawcy

http://www.elsevier.com