Structure of dihydroxyacetone phosphate dimethyl acetal, a stable dihydroxyacetone phosphate precursor, in the crystalline state.

Autorzy

Katarzyna Ślepokura

Tadeusz Lis

Rok wydania

2006

Czasopismo

Carbohydrate Research

Numer woluminu

341

Strony

507-524

DOI

10.1016/j.carres.2005.12.003

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Crystal and molecular structures of four different salts of a dihydroxyacetone phosphate (DHAP) precursor, its dimethyl acetal [2,2-dimethoxy-1,3-propanediol phosphate, C(5)H(13)O(7)P, (MeO)(2)DHAP]: (cha)(2)[(MeO)(2)DHAP].H(2)O (6a), (cha)[(MeO)(2)DHAP] (6b), Na(2)[(MeO)(2)DHAP].5.75H(2)O (6c) and K(2)[(MeO)(2)DHAP].H(2)O (6d), along with the cyclohexylammonium (cha) salt of its phenyl ester (cha)[(MeO)(2)DHAP(Ph)] (6e) are described. In the (MeO)(2)DHAP mono- and dianions, slightly different orientation of the phosphate group in relation to the acetal carbon atom is observed, with a delicate tendency of phosphate group to be located antiperiplanar in the monoanions and anticlinal in the dianions. The 2,2-dimethoxy-1,3-propandiol moiety, (MeO)(2)DHA, seems to be very rigid and its conformation is independent of phosphorylation, the ionization state of the inserted phosphate group and its additional substitution. The overall structures of the cyclohexylammonium (6a,b) and potassium salts (6d) have a double-layered architecture, while the sodium cation network in 6c forms the system of channels, which are filled up with the [(MeO)(2)DHAP](2-) ions. The different architectures of 6c and 6d crystals result from the different ways in which the relevant dianions coordinate to sodium and potassium ions and affect also the hydrogen bonding system observed in 6c and 6d crystals.

Słowa kluczowe

Sugar phosphates, Dihydroxyacetone phosphate (DHAP) precursor, Dihydroxyacetone phosphate (DHAP) dimethyl acetal, Sodiumpotassium coordination, O–H···O, N–H···O, C–H···O hydrogen bonds