# Structure of cyclic dihydroxyacetone phosphate dimethyl acetal, a cyclic DHAP precursor, in the crystalline state.

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Rok wydania

2008

Czasopismo

Carbohydrate Research

Numer woluminu

343

Strony

113-131

DOI

10.1016/j.carres.2007.09.011

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The six-membered cyclic phosphate diester, 5,5-dimethoxy-2-oxo-1,3,2-dioxaphosphorinane-2-ol, the dimethyl acetal of cyclic dihydroxyacetone phosphate, $(MeO)_2$cDHAP, was obtained by the isolation of an intermediate in the basic hydrolysis of the cyclic triester derivative. The compound had been isolated in the form of the crystalline cyclohexylammonium (cha) salts: (cha)[$(MeO)_2$cDHAP]·3$H_2O$ (**5a**) and (cha)[$(MeO)_2$cDHAP]·$H_2O$ (**5b**), which were then converted into the free acid: ($H_5O_2$)[$(MeO)_2$cDHAP] (**5c**) and then into a series of different salts: Na[$(MeO)_2$cDHAP]·2$H_2O$ (**5d**), K[$(MeO)_2$cDHAP]·1.5$H_2O$ (**5e**), K[$(MeO)_2$cDHAP]·0.5$H_2O$ (**5e′**), Ca[$(MeO)_2$cDHAP]$_2$·2$H_2O$ (**5f**), CaK[$(MeO)_2$cDHAP]$_3$·2$H_2O$ (**5g**) and $NH_4$[$(MeO)_2$cDHAP] (**5h**). The synthesis of the compounds, their crystallization and crystal structures determined by X-ray crystallography are described. The most interesting structural feature observed in **5a**–**g** anions in the crystalline state is the chair conformation of the P/O/C/C/C/O 1,3,2-dioxaphosphorinane ring, which is generally not flattened, in contrast to the deformations often observed in the analogous aryl derivatives (also in $(MeO)_2$cDHAP(Ph); Ślepokura, K.; Lis, T. *Acta Crystallogr. Sect. C* **2004**, *60*, o315–o317). However, the anion in crystal **5h** is disordered and exists in two conformations, 76% of which is the skew, *S*, conformation, not observed so far in the compounds of related structure.

Słowa kluczowe

Cyclic phosphates, cDHAP, Cyclic dihydroxyacetone phosphate dimethyl acetal, atom, Ion, 2-Dioxaphosphorinane ring, X-ray crystal structure

Adres publiczny

https://doi.org/10.1016/j.carres.2007.09.011