Structure of two isomers of 2,5-diethoxy-2,5-bis(hydroxymethyl)-[1,4]-dioxane at 100 K.

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2003

Czasopismo

Journal of Molecular Structure

Numer woluminu

647

Strony

223-231

DOI

10.1016/S0022-2860(02)00529-X

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The crystal and molecular structures of the *cis*- and *trans*-isomers of 2,5-diethoxy-2,5-bis(hydroxymethyl)-[1,4]-dioxane have been determined by X-ray analysis. The *cis*- (**I**) and *trans*-isomers (**II**) crystallize in the monoclinic (space group $P2_1/c$) and orthorhombic (*Pbca*) system, respectively. The [1,4]-dioxane ring of the *cis*-isomer molecule adopts a twist-boat conformation, while the ring of the *trans*-isomer is a chair. The two ethoxy groups in **II** are in more crowded axial positions, due to the anomeric effect. The anomeric effect, stronger in the *cis*-isomer, influences its stability, despite the presence of two bulky hydroxymethyl groups in the equatorial orientation and the low-energy chair conformation of the *trans*-isomer. Both hydroxyl groups in **I** and **II** act as donors in intermolecular two-centre and three-centre O–H···O hydrogen bonding, which may be classified as medium strong and weak. Additionally, there are C–H···O hydrogen interactions in each crystal; that in the *cis*-isomer is intramolecular.

Słowa kluczowe

Twist-boat conformation, [1, 4]-Dioxane ring, Intermolecular hydrogen bonds, Three-centre hydrogen bonds, Weak C–H···O intermolecular contacts

Adres publiczny

https://doi.org/10.1016/S0022-2860(02)00529-X

Strona internetowa wydawcy

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