

X-Ray diffraction and quantum-chemical analysis of a single crystal of 2,5-dimethyl-3,4-dihydro-2H-pyran-2-carboxylic acid.

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Rok wydania

2011

Czasopismo

Chemistry of Heterocyclic
Compounds

Numer woluminu

46

Strony

1443-1448

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The structure of synthesized 2,5-dimethyl-3,4-dihydro-2H-pyran-2-carboxylic acid was investigated by the single crystal X-ray diffraction analysis method. It was established that the molecule of the acid exists in the form of the endo isomer while the single crystal exists as a racemate of the two enantiomeric endo stereomers. Quantum-chemical calculations of a model of the macrocell of the acid by means of the semiempirical MOPAC2009 program agree well with the X-ray diffraction data. Keywords: 2,5-dimethyl-3,4-dihydro-2H-pyran-2-carboxylic acid, quantum-chemical calculations, MOPAC2009, RM1, single crystal X-ray diffraction analysis, Winmostar. Pyran derivatives and the dimers of acrolein and its homologs in particular are valuable starting substances for the synthesis of dyes, plasticizers, surface-active substances, fungicides, insecticides, and drugs [1]. The dimers of α -alkylacroleins are synthesized by the Diels–Alder reaction, and their subsequent disproportionation in an alkaline medium by the Cannizzaro reaction leads to the formation of oxidation products (the salts of pyrancarboxylic acids) and reduction products (pyran alcohols) [2]. O

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