

Solid state and solution behaviour of *N*-(2-pyridyl)- and *N*-(4-methyl-2-pyridyl)aminomethane-1,1-diphosphonic acids.

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Rok wydania

2006

Czasopismo

Journal of Molecular
Structure

Numer woluminu

782

Strony

81-93

DOI

10.1016/j.molstruc.2005.07.004

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The crystal structures of *N*-(2-pyridyl)aminomethane-1,1-diphosphonic acid (**1**) and *N*-(4-methyl-2-pyridyl)aminomethane-1,1-diphosphonic acid (**2**) are determined and discussed with respect to their geometry and solid state organization. Compounds **1** and **2** crystallize as the opposite *E* and *Z* isomers. However, in solution both appear as a mixture of the *Z* and *E* forms. From the temperature dependence of NMR spectra, the *Z/E* ratio is assigned to be nearly equal in **1** and 0.69:0.31, respectively, in **2**. The role of a substituent position on the pyridyl ring for the *Z/E* ratio in solution and for solid state conformations of *N*-(2-pyridyl)aminomethane-1,1-diphosphonic acids is discussed as well.

Słowa kluczowe

Bisphosphonates, Self-assembly, Hydrogen bonds, X-ray diffraction, Dynamic NMR spectroscopy

Adres publiczny

<https://doi.org/10.1016/j.molstruc.2005.07.004>

Strona internetowa wydawcy

<http://www.elsevier.com>