

Conformational isomers of the [5-methyl-2-pyridinio)aminomethylene]diphosphonate dianion and [(5-methyl-2-pyridyl)aminomethylene]-diphosphonate trianion in salts with 4-aminopyridine and ammonia.

Autorzy

Ewa Matczak-Jon

Katarzyna Ślepokura

Paweł Kafarski

I. Skrzyńska

Marek Jon

Rok wydania

2009

Czasopismo

Acta Crystallographica

Section C: Structural

Chemistry

Numer woluminu

C65

Strony

261-266

DOI

10.1107/S0108270109010683

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The crystal structures of two salts, products of the reactions between [(5-methyl-2-pyridyl)aminomethylene]bis(phosphonic acid) and 4-aminopyridine or ammonia, namely bis(4-aminopyridinium) hydrogen [(5-methyl-2-pyridinio)aminomethylene]diphosphonate 2.4-hydrate, $2C(5)H(7)N(2)(+).C(7)H(10)N(2)O(6)P(2)(2-).2.4H(2)O$, (I), and triammonium hydrogen [(5-methyl-2-pyridyl)aminomethylene]diphosphonate monohydrate, $3NH(4)(+).C(7)H(9)N(2)O(6)P(2)(3-).H(2)O$, (II), have been determined. In (I), the Z configuration of the ring N-C and amino N-H bonds of the bisphosphonate dianion with respect to the C(ring)-N(amino) bond is consistent with that of the parent zwitterion. Removing the H atom from the pyridyl N atom results in the opposite E configuration of the bisphosphonate trianion in (II). Compound (I) exhibits a three-dimensional hydrogen-bonded network, in which 4-aminopyridinium cations and water molecules are joined to ribbons composed of anionic dimers linked by O-H...O and N-H...O hydrogen bonds. The supramolecular motif resulting from a combination of these three interactions is a common phenomenon in crystals of all of the Z-isomeric zwitterions of 4- and 5-substituted (2-pyridylaminomethylene)bis(phosphonic acid)s studied to date. In (II), ammonium cations and water molecules are linked to chains of trianions, resulting in the formation of double layers.

Adres publiczny<http://doi.org/10.1107/S0108270109010683>

