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Conformations and resulting hydrogen-bonded networks of hydrogen {phosphono[pyridin-1-ium-3-yl)amino]methyl}phosphonate and related 2-chloro and 6-chloro derivatives.

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Streszczenie

In the crystal structures of the conformational isomers hydrogen {phosphono[(pyridin-1-ium-3-yl)amino]methyl}phosphonate monohydrate (pro-E), C(6)H(10)N(2)O(6)P(2)·H(2)O, (Ia), and hydrogen {phosphono[(pyridin-1-ium-3-yl)amino]methyl}phosphonate (pro-Z), C(6)H(10)N(2)O(6)P(2), (Ib), the related hydrogen {[(2-chloropyridin-1-ium-3-yl)amino] (phosphono)methyl}phosphonate (pro-E), C(6)H(9)ClN(2)O(6)P(2), (II), and the salt bis(6-chloropyridin-3-aminium) [hydrogen bis({[2-chloropyridin-1-ium-3-yl(0.5+)]amino}methylenediphosphonate)] (pro-Z), 2C(5)H(6)ClN(2)(+)·C(12)H(16)Cl(2)N(4)O(12)P(4)(2-), (III), chain-chain interactions involving phosphono (-PO(3)H(2)) and phosphonate (-PO(3)H(-)) groups are dominant in determining the crystal packing. The crystals of (Ia) and (III) comprise similar ribbons, which are held together by N-H···O interactions, by water- or cation-mediated contacts, and by π-π interactions between the aromatic rings of adjacent zwitterions in (Ia), and those of the cations and anions in (III). The crystals of (Ib) and (II) have a layered architecture: the former exhibits highly corrugated monolayers perpendicular to the [100] direction, while in the latter, flat bilayers parallel to the (001) plane are formed. In both (Ib) and (II), the interlayer contacts are realised through N-H···O hydrogen bonds and weak C-H···O interactions involving aromatic C atoms.

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