

Structural landscape studies of aminopyridinium hypodiphosphates: dehydration and polymorphism in 4-aminopyridinium salts

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Streszczenie

A series of 4-aminopyridinium (4ap) hypodiphosphates has been synthesized and characterized by variable temperature (VT) optical microscopy, thermogravimetry (TGA-DSC) and X-ray diffraction techniques (SC-XRD, PXRD, VT μ -PXRD). Anhydrous salts (4apH)(H₃P₂O₆) (**2**) and (4apH)₂(H₂P₂O₆) in monoclinic (*C2/c*) (**4**), orthorhombic (*P*₂₁2₁2₁) (**5**) and another monoclinic (*Cc*) (**6**) polymorphic modifications were obtained by single crystal-to-powder dehydrations of the hydrates: ionic co-crystal (4apH)₂(H₂P₂O₆)·H₄P₂O₆·2H₂O (**1**) and salt (4apH)₂(H₂P₂O₆)·2H₂O (**3**), respectively. Compound (**2**) was the only anhydrous form which was also obtained by a typical solution-crystallization. Destructive dehydrations strongly affected hypodiphosphate substructures, generating new structural motifs (both in PP–PP and ap–PP interactions) and new crystal architectures, thus revealing the structural diversity in organic hypodiphosphates. Dehydration gave rise to new properties, as non-centrosymmetric and polar anhydrous structures, (**5**) and (**6**) respectively, were obtained from centrosymmetric hydrate (**3**).

Adres publiczny

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