Synthesis, crystal structure and Hirshfeld surface analysis of acidic salt [4-methyl phenyl ammonium][O-phenyl](hydroxyl)phosphate, [4-CH₃-C₆H₄NH₃][C₆H₅O]P(O)(O)(OH)

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(Received: 22/5/2016 , in revised form: 29/8/2016 )

Abstract: The synthesis and X-ray diffraction analysis of a new acidic salt, [4-methyl-phenyl ammonium][O-phenyl](hydroxyl)phosphate, [4-CH₃-C₆H₄NH₃][C₆H₅O]P(O)(O)(OH), is reported. This compound crystallizes in the monoclinic system, with space group P2₁/c (a = 9.5147(4) Å, b = 23.2158(10) Å, c = 13.2740(6) Å and β = 111.244(4)°) with four independent components including two cations and two anions in the asymmetric unit. In the crystal, adjacent components are linked together through N–H⋯O and O–H⋯O hydrogen bonds building a ladder arrangement along [100] axis. The Hirshfeld surface analysis and two-dimensional fingerprint plot were used to study intermolecular interactions in the structure. The N–H⋯O and O–H⋯O hydrogen bonds are the characteristic interactions (red areas in the Hirshfeld surfaces). Two sharp spikes in the fingerprint plots of two anions are related to the O⋯H(O) contacts, while one nearly sharp spike in the fingerprint of two cations is assigned to the O⋯H(N) contacts.

Keywords: Acidic salt [4-methyl phenyl ammonium][O-phenyl](hydroxyl)phosphate; X-ray diffraction analysis; hydrogen bonding; Hirshfeld surface analysis.

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