Formation and Crystal Structure of 2,3,5-Triphenyltetrazolium Hexachlorophosphate and Dichlorophosphate(V), [TPT]+[PCl₆]⁻ and [TPT]+[PO₂Cl₂]⁻

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2,3,5-Triphenyltetrazolium hexachlorophosphate, [C₁₉H₁₅N₄]⁺[PCl₆]⁻, [TPT]⁺[PCl₆]⁻ (1), and 2,3,5-triphenyltetrazolium dichlorophosphate(V), [C₁₉H₁₅N₄]⁺[PO₂Cl₂]⁻, [TPT]⁺[PO₂Cl₂]⁻ (2), were synthesized by reactions of anhydrous 2,3,5-triphenyltetrazolium chloride, [TPT]⁺Cl⁻, and 2,3,5-triphenyltetrazolium chloride monohydrate [TPT]⁺Cl⁻·H₂O, with PCl₅ in dry acetonitrile, and their crystal structures were determined by single-crystal X-ray diffraction analysis. In the title compounds, the [TPT]⁺ cations show a face-to-face stacked orientation between the phenyl rings of neighboring molecules, which is caused by intermolecular π···π interactions. The crystal structure of compound 1 consists of layers of 2,3,5-triphenyltetrazolium cations and hexachlorophosphate anions. In compound 2 the tetrahedral [PO₂Cl₂]⁻ anions exhibit approximate C₂ᵥ symmetry with P–O bond lengths from 1.454 to 1.463 Å and P–Cl bond lengths from 2.038 to 2.050 Å. The Raman spectrum of compound 1 was recorded, and the assignment of the [PCl₆]⁻ Raman modes is proposed.

Key words: 2,3,5-Triphenyltetrazolium Hexachlorophosphate(V), 2,3,5-Triphenyltetrazolium Dichlorophosphate(V), [PCl₆]⁻, [PO₂Cl₂]⁻, Crystal Structure, Raman Spectroscopy