Reactivity of Tetramethylphosphonium Fluoride in Acetonitrile Solutions

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Anhydrous tetramethylphosphonium fluoride dissolved in acetonitrile reacts slowly with the solvent under formation of (*E*)-2-amino-1-cyano-propene which was characterized by infrared and NMR spectroscopy. An attempted preparation of $[Me_3PF_3]^-$ by addition of Me_3PF_2 to Me_4PF/acetonitrile solutions has shown that the desired reaction does not occur, but prolonged reaction times and small acetonitrile concentrations lead to the formation of the iminophosphorane $Me_3P{=}NC(Me){=}CH_2$ and $[Me_4P]^+HF_2{}^-$. $Me_3P{=}NC(Me){=}CH_2$ was characterized by infrared spectroscopy and a single-crystal structure determination. *N*-(2-propenyl)trimethyliminophosphorane crystallizes in the monoclinic space group $P2_1/c$ with a = 1006.8(2), b = 1523.5(3), c =1180.3(2) pm, β = 111.72(6)° and Z = 8. The two independent molecules per unit cell have nearly planar P=N-C(C)=C skeletons with torsion angles P–N–C–C of 5.9(3)° and 7.1(4)° and an average P=N distance of 158.1(2) pm. The general ability of Me_4PF as a fluoride donor was proven by the reaction with SO_2 which results in the formation of $[Me_4P]^+SO_2F^-$. The colorless salt was characterized by infrared, Raman, and NMR spectroscopy.

Key words: Iminophosphorane, Vibrational Spectroscopy, NMR Spectroscopy, Crystal Structure