Carbacylamidophosphates: Synthesis and Structure of N,N'-Tetramethyl-N''-benzoylphosphoryltriamide and Dimorpholido-N-benzoylphosphorylamide

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N,N'-Tetramethyl-N''-benzoylphosphoryltriamide (I) and dimorpholido-N-benzoylphosphorylamide (II), and their sodium salts NaI, NaII were synthesized and characterized by means of IR and 1H, 31P NMR spectroscopy. The structures of I, II were determined by X-ray diffraction:

I monoclinic, space group P21/c with \(a = 10.162(3)\), \(b = 11.469(4)\), \(c = 12.286(4)\) Å, \(\beta = 94.04^\circ\), \(V = 1428.4(8)\) Å\(^3\), \(Z = 4\), \(\rho_{\text{calcld.}} = 1.187\) g/cm\(^3\);

II monoclinic, space group C2/c with \(a = 15.503(4)\), \(b = 10.991(3)\), \(c = 22.000(6)\) Å, \(\beta = 106.39^\circ\), \(V = 3596.3(17)\) Å\(^3\), \(Z = 8\), \(\rho_{\text{calcld.}} = 1.253\) g/cm\(^3\). The refinement of the structures converged at \(R = 0.0425\) for I, and \(R = 0.068\) for II. In both structures the molecules are connected into centrosymmetric dimers via hydrogen bonds formed by the phosphoryl oxygen atoms and hydrogen atoms of amide groups.