

Carbacylamidophosphates: Structure and Properties of Bis(N,N'-morpholido)-[(N''-morpholido)-carboxamido] phosphate

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The bis(N,N'-morpholido)-[(N''-morpholido)-carboxamido] phosphate: O(CH₂CH₂)NC(O)-N(H)P(O)[N(CH₂CH₂)O]₂ [HL], has been prepared and characterized by means of IR, ³¹P and ¹H NMR spectroscopy and X-ray diffraction (triclinic, $a = 9.282(2)$, $b = 9.308(2)$, $c = 21.341(4)$ Å, $\alpha = 80.79(3)^\circ$, $\beta = 80.92(3)^\circ$, $\gamma = 66.92(3)^\circ$, $V = 1665.1(6)$ Å³, space group P $\bar{1}$, $Z = 4$ and $R = 0.0423$, $wR2 = 0.1303$ for 6774 unique reflections used). The unit cell consists of two independent molecules connected by hydrogen bonds N-H...O=P into non-symmetric dimers. The compound behaves as a HL molecule with a protonation constant corresponding to the -C(O)N(H)P(O)- group of $pK = 8.65$ as determined by potentiometric studies.