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

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Carbacylamidophosphates, X-Ray Data, NMR Data

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, \( \alpha = 80.79(3) \), \( \beta = 80.92(3) \), \( \gamma = 66.92(3) \)), \( V = 1665.1(6) \) Å³, space group \( \text{P} \bar{1} \), \( Z = 4 \) and \( R = 0.0423 \), \( wR = 0.1303 \) 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.