The Double Hydrogen Bond Acceptor Capability of Phosphoryl Oxygen Atom in $C_6H_5P(O)[NHC_6H_4\text{-}4\text{-}CH_3]_2$

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In the structure of bis(4-methylphenylamido) phenylphosphine oxide, $C_6H_5P(O)[NHC_6H_4\text{-}4\text{-}CH_3]_2$, the O atom of P═O group acts as a double H-bond acceptor, resulting from the involvement of two H-atom donor sites (N—H units) with one H-atom acceptor site (P═O group), in the hydrogen-bonding interactions. So, in the crystal packing, adjacent molecules are linked *via* $(N—H)_2…O═P$ hydrogen bonds into linear arrangements parallel to [010] by forming $R_2^1(6)$ rings. The observation in the title amido-phosphine oxide, with a $(C)P(═O)(NH)_2$ skeleton, is similar to what was found, through a Cambridge Structural Database [1] analysis, for the phosphoramide compounds with a higher number of H-atom donor sites relative to H-atom acceptor sites in molecules with $P(═O)(NH)_3$, $(N)P(═O)(NH)_2$, $C(═O)NHP(═O)(NH)_2$ and $(NH)_2P(═O)OP(═O)(NH)_2$ groups, or in some compounds with the remarkable H-atom acceptor capability of the phosphoryl oxygen atom relative to the other acceptor center in the molecule, for example in molecules with an $(O)P(═O)(NH)_2$ skeleton [2]. In the title phosphine oxide, the environment at the nitrogen atom is almost planar and it does not take part in hydrogen bonding as an acceptor, reflecting its low Lewis base character. The compound was also characterized by elemental analysis, melting point, $^{31}P\{^1H\}$, ^1H, ^{13}C NMR, UV-Visible and IR.

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References:

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