Supramolecular architecture of $((C_6H_5CH_2)_2N)(C_6H_4)(NH)_2P(O)$

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Phosphoric triamides are well-known for their biological activities and some other applications as extractant, solvent and ligand [1]. The crystal structure of a new diazaphosphole-holding phosphoric triamide with the formula $((C_6H_5CH_2)_2N)(C_6H_4)(NH)_2P(O)$ is studied (**Figure**). The P—N bond made by the $(C_6H_5CH_2)_2N$ moiety is slightly shorter than the P—N bonds of diazaphosphole ring. The benzyl moieties adopt the +*ac*–*sc*+*ac*+*sp* and +*ac*–*sc*+*ac*+*ap* conformations (*ac* = anticlinal, *sc* = synclinal, *sp* = synperiplanar, *ap* = antiperiplanar), based on the 2×C—C—C—N/C—C—N—P/C—N—P=O torsion angles. In the crystal structure, the molecules are aggregated through N—H…O=P hydrogen bonds in a tape arrangement along the *a* axis. This assembly includes centrosymmetric eight-membered ring hydrogen bond motifs, in which the P=O group takes part as a double-hydrogen bond acceptor. The C—H…π interactions extend the supramolecular assembly to a two-dimensional array parallel to the *ab* plane.

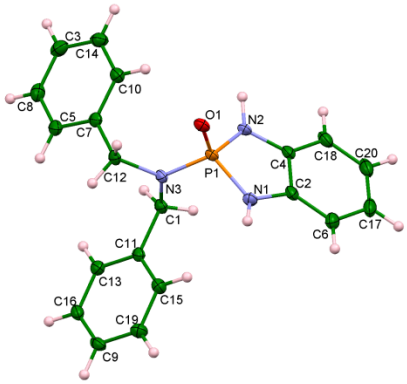

Figure: The molecular structure, showing the atom-numbering scheme for the title compound, with displacement ellipsoids drawn at the 50% probability level.

References

[1] Corbridge, D. E. C. In Phosphorus: An Outline of Its Chemistry, Biochemistry and Technology, 5th ed. Amsterdam: Elsevier, 1995.