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Synthesis, spectroscopic characterization and crystal structure of a new chiral amidophosphoester

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Abstract:

The chiral amidophosphoester families have found widespread use in the preparation of different classes of drugs, and for processing of biologically active compounds [1]. We report here the synthesis of single-enantiomer amidophosphoester (C₆H₅O)₂P(O)[(R)-(+)-NHCH(CH₃)(C₆H₄-4-CH₃)] (I) and its characterization by IR, NMR, mass, optical rotation and single crystal X-ray diffraction. The compound crystallizes in monoclinic system with chiral space group *P*2₁. The asymmetric unit is composed of two independent molecules. The P atoms have a distorted tetrahedral (O)₂P(O)(N) configuration. In the crystal, chiral one-dimensional hydrogen-bonded architecture, formed along *b* axis, is mediated by classical N—H...O(P) and weak C—H...O(P) hydrogen bonds. This architecture includes *D*₁¹(2), *R*₂²(10), *C*₂²(8) and *C*₂¹(8) graph-set motifs. In the IR spectrum, the band centered at 3174 cm⁻¹ is attributed to the NH stretching frequency. The melting point of title structure (393 K) is a few lower than the closely related analogous compound (C₆H₅O)₂P(O)[(R)-(+)-NHCH(CH₃)(C₆H₅)]₂ (408 K) [2]. The phosphorus signal appears at -0.07 ppm, in comparison with the signal at -0.81 ppm for this analogous compound noted [2]. The two diastereotopic phenyl groups reveal two sets of signals in ¹H- and ¹³C{¹H}-NMR spectra. The specific optical rotation is measured as [α]_D²⁰ = 51° (*c* 0.009, MeOH).

References:

- [1] Warren, T. K., *et al.* (2016). *Nature*, **531**, 381–385.
- [2] Sabbaghi, F., Pourayoubi, M., Nečas, M., Damodaran, K. (2019). *Acta Cryst. C* **75**, 77–84.