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Two single-enantiomer (R and S) Amidophosphoesters

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The compound $(C_6H_5O)_2P(O)[NHCH(CH_3)(C_6H_5)]$ exists in previously published papers, with together its melting point, elemental analysis and selected mass spectrum peaks, and with no sign of the type of $NHCH(CH_3)(C_6H_5)$ fragment as R, S or racemic. Here, the crystal structures of $(C_6H_5O)_2P(O)[NH(+)CH(CH_3)(C_6H_5)]$ and $(C_6H_5O)_2P(O)[NH(–)CH(CH_3)(C_6H_5)]$ are reported. The compounds are named as diphenyl (R-(+)-α-methylbenzylamido)phosphate, (I), and diphenyl (S-(–)-α-methylbenzylamido)phosphate, (II). In both structures, the chiral one-dimensional hydrogen-bonded architectures, along [010], are built from NH…OP interactions; however, they are mirror images of each other. The assemblies of these compounds include the non-centrosymmetric graph-set motif *C*(4) and the compounds crystallize in the chiral space group $P2_1$. Figure 1 shows the assembly of the structure (II), for a typical example. For each molecule, the two C_6H_5O groups bonded to phosphorus are different in NMR media (monitored by ^1H and ^{13}C NMR). For both compounds, the phosphorus signal exactly appears at –0.81 ppm (DMSO-d_6), in a calibrated condition (concentration, temperature).

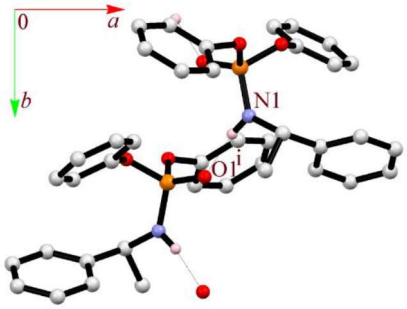

Fig. 1 A partial view of crystal packing of (II) showing the linear hydrogen bond pattern along the *b* axis. The N—H...O hydrogen bonds are shown as dotted lines. The C-bound H atoms have been omitted for clarity.

References

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