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Synthesis, NMR spectroscopic characterization and *X*-ray crystallographyof (R, S)–$(C_5H_9NH)P(O)(OC_6H_5)(NHC_6H_4$-$p$-$CH_3)$ and (R, S)–$(4$-$CH_3C_5H_9N)P(O)(OC_6H_5)(NHC_6H_4$-$p$-$CH_3)$

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In continuation of the previous works on synthesis and structure determination of racemate mixed-amidophosphinates with $(N^2)P(O)(O)(N^1)$ skeleton [1-4], two new rac-$XP(O)(OC_6H_5)(NHC_6H_4$-p-$CH_3)$ [X = NHC_5H_9 (1) and $N(4$-$CH_3C_5H_9)$ (2)] mixed amidophosphinates were synthesized and characterized by $^{31}P\{^1H\}$, ^{13}C, ^1H NMR spectroscopy and single crystal X-ray determination. The P atom in each molecule is in a distorted tetrahedral environment with two different amido groups bonded to P atom [1-4]. The asymmetric unit of 1 and 2 are composed of one molecule and two symmetrically independentmolecules, respectively. Among the two independent molecules in the asymmetric unit of (2), one C_6H_5O group was found to be disordered. In the structures, the oxygen atom of C_6H_5O group and the nitrogen atoms bonded to P do not take part in hydrogen bonding as an acceptor; whereas, the oxygen atom of phosphoryl acts as a double-H bond acceptor. Adjacent molecules are linked via N—H···O=P hydrogen bonds in a linear arrangement, parallel to [010] for (1) and [100] for (2).

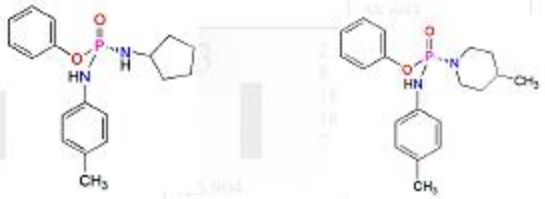

Fig. 1. The chemical structures of (1) and (2)are shown.

References

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