

**Synthesis and characterization of some new phosphoramidate and
thiophosphoramidate derivatives: crystal structure of
CHCl₂C(O)NHP(O)[NHCH₂CH₂CH₃]₂**

Mehرداد Pourayoubi^{a,*}, Ehteram Mohammadi Gooshki^a, Mohammad Abad^a, Marek Nečas^{b,c}

^aDepartment of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran

^bDepartment of Chemistry, Masaryk University, Kotlarska 2, 61137 Brno, Czech Republic,

^cCEITEC - Central European Institute of Technology, Masaryk University, Kamenice 5, 62500 Brno, Czech Republic, (e-mail: pourayoubi@um.ac.ir)

A new phosphoric triamide structure, CHCl₂C(O)NHP(O)[NHCH₂CH₂CH₃]₂ (i), is investigated. The P atom is within an [N_{CP}]P(O)[N]₂ environment (N_{CP} is the nitrogen atom of the C(O)NHP(O) segment) with the bond angles at the P atom in the range of 103.46(9) to 118.51(9)°. The N_{CP}—H bond adopts a *syn* conformation with respect to the P=O group, whereas, the two other N—H units are in an *anti* conformation with respect to the P=O group. As it is expected and observed for analogous structures,¹ the P—N_{CP} bond length (of 1.6962(16) Å) is longer than the two other P—N bonds (1.6201(16) and 1.6257(18) Å). In the crystal structure, molecules are aggregated in a one-dimensional arrangement parallel to the plane (1–10) in the direction perpendicular to the (110) plane (Fig. 1). The spectroscopic features of the title structure as well as some phosphoramidates ([2-Cl-C₆H₄O]P(O)[NHCH₂C₆H₄-4-Cl]₂ (ii), [2-Cl-C₆H₄O]P(O)[NHCH₂C₆H₄-4-CH₃]₂ (iii), [4-Cl-C₆H₄CH₂NH]₃P(O) (iv)) and thiophosphoramidates ([4-Cl-C₆H₄CH₂NH]₃P(S) (v), [4-CH₃-C₆H₄CH₂NH]₃P(S) (vi), [CH₃O]₂P(S)[NHCH₂C₆H₄-4-CH₃]₂ (vii)) are reported.

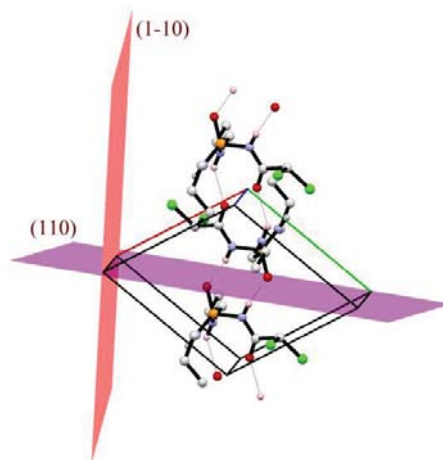


Fig. 1. A view of the crystal packing of CHCl₂C(O)NHP(O)[NHCH₂CH₂CH₃]₂ is represented. The carbon-bound H atoms were omitted for the sake of clarity and the hydrogen bonds are shown as dotted lines.

References

- 1 M. Toghraee, M. Pourayoubi, V. Divjakovic, *Polyhedron*, 2011, **30**, 1680–1690.