



**Synthesis and Crystal structure of a New N-(2,6-dichlorobenzoyl)-  
N',N',N'',N''-tetra(ethyl)-Phosphoric triamide**

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Organophosphorus compounds are well-known as the biologically active substances [1]. Among them the anticancer activity of compounds having a C(O)NHP(O) skeleton has been studied [2]. In a recently published paper, patterns of hydrogen bonds in phosphoric triamides containing a C(O)NHP(O) skeleton have been discussed [3]. The synthesis and X-ray crystal structure of the title phosphoric triamide is a continuation of work on this family of compounds in our laboratory. Following our previous works about C(O)NHP(O)-based phosphoric triamides such as P(O)[NHC(O)CHCl<sub>2</sub>][N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub> [3], here, the synthesis, spectroscopic characterization (by <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P NMR, IR) and crystal structure of 2,6-Cl<sub>2</sub>-C<sub>6</sub>H<sub>3</sub>C(O)NHP(O)[N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub> are reported. Single crystals of title compound were obtained from a solution of CH<sub>3</sub>OH and CH<sub>3</sub>CN after slow evaporation at room temperature. The asymmetric unit contains four symmetrically independent molecules. In each molecule, the P—N bond lengths in the P(O)[N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub> fragment are shorter than the other P—N bond. The P=O bond lengths of 1.477(3) Å for P1, 1.482(3) Å for P2, 1.479(3) Å for P3 and 1.479(3) Å for P4 are longer than the normal P=O bond length (1.45 Å). The phosphorus atoms have a disordered tetrahedral configuration; the bond angles at the P atoms are in the range of 105.20(15)°-115.88(16)° for molecule P1, 104.99(15)°-115.71(17)° for P2, 105.37(15)°-115.72(17)° for P3 and 105.44(16)°-114.46(18)° for P4. In the crystal packing, two independent dimers are formed through intermolecular P=O...H—N hydrogen bonds, as R<sub>2</sub><sup>2</sup>(8) rings.

**References:**

- [1] F. Ekstrom, C. Akfur, A. Tunemalm, S. Lundberg, *Biochemistry* 45 (2006) 74.
- [2] K. Gholivand, N. Dorosti, Z. Shariatinia, F. Ghaziany, S. Sarikhani, M. Mirshahi, *Med. Chem. Res.* 20 (2011) 1287.
- [3] M. Toghraee, M. Pourayoubi, V. Divjakovic, *Polyhedron* 30 (2011) 1680.