



پانزدهمین کنفرانس علمی ایران ۱۳-۱۵ شهریور ۱۳۸۶ - مشهد و مریز



R¹=Cl, H
R²=Cl, MeO

Reference

- [1] KS sharma, SP Singh, Indian J Chem, 31B, (1992), 396.
- [2] I Lalezari, A Shafiee, J. Khorrami, A. Soltani, J. Pharm. Sci. 67,(1987)1336-1338
- [3] D.L. Klayman, W.H.H. Gunther, Organic Selenium Compounds their Chemistry and Biology, Washington, New York, (1972), 731

Crystal structure and H-bond pattern of a new acetyl phosphorylamidate

A. Tarahhomi^{a,*}, M. Pourayoubi^a

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran

E-mail: tarahhomi_at@yahoo.com

Acetyl phosphorylamidates, with the general formula R¹C(O)NHP(O)R² have been attracted attention due to containing nitrogen-carbonyl and nitrogen-phosphoryl moieties, and special properties resulting from them such as acting as O, O'-donor ligands [1] and inhibitory of urease and acetylcholinesterase enzymes [2].

The new compound 5,5-dimethyl-2-[N-(2,6-difluorobenzoyl)]-2-oxo-1,3,2-diazaphosphorinane was synthesized and characterized by ¹H, ¹³C, ³¹P(¹H)-NMR and IR spectroscopy and single crystal X-ray determination. The P atoms have a distorted tetrahedral configuration with the bond angles O(2)-P(1)-N(2) 115.27(14)°, O(2)-P(1)-N(3) 115.57(16)°, N(2)-P(1)-N(3) 103.67(15)°, O(2)-P(1)-N(1) 109.55(14)°, N(2)-P(1)-N(1) 108.12(16)° and N(3)-P(1)-N(1) 103.79(14)°, the phosphoryl and carbonyl groups are *gauche* to each other. In this structure, the intermolecular P=O...H—N_{C(O)NHP(O)} and C=O...H—N_{amide} HBs are responsible to connection of the molecules together as 1-D chains. Moreover, co-crystallization of solvent molecule (CH₃OH) was occurred in the structure via P=O...H-OCH₃ (O...O = 2.714(3) Å) and CH₃(H)O...H-N_{amide} (O...N = 2.904(4) Å) HBs along this chain. Therefore, each molecule is hydrogen-bonded to two molecules of CH₃OH. Another interesting feature of this structure is the existence of C—H...O HBs that provide R₃²(13), R₂²(9) and R₃²(9) rings. In addition to, the combinations of the C—H...F and the C—H...O HBs make the R₂²(10) and R₃²(9) rings. These HBs expanded the crystal structure into a 3-D arrangement.

Reference

- [1] Gholivand K., Mostanzadeh H., Koval T., Dusek M., Erben M. F., Stoeckli-Evans H., Della Vedova C. O. (2010) *Acta Cryst.* B66, 1-10.
- [2] Gholivand K., Shariatnia Z., Khajeh K., Naderimaneh H. (2006) *Journal of Enzyme Inhibition and Medicinal Chemistry* 21 (1), 31-35.

Synthesis and crystal structure of N-(2-fluorobenzoyl)-N',N''-diisopropylphosphoric triamide

A. Tarahhomi^{a,*}, M. Pourayoubi^a

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran

E-mail: tarahhomi_at@yahoo.com

Recently, the chemistry of phosphoramidates has been considered due to their antiviral and anticancer activities [1], their coordination chemistry [2] and having a decisive role in catalytic and metabolism processes [3]. Phosphoramidates of the general formula RC(O)NHP(O)X₂, are potential O, O'-donor ligands for metal complexation, particularly for lanthanide ions.

Following the previous works about carbacylamidophosphates with a C(=O)NHP(=O) skeleton such as P(O)[NHC(O)C₆H₄(4-F)][HNC₆H₄CH₃]₂ [4] and P(O)[NHC(O)C₆H₃(2,6-F₂)][HNC(CH₃)₃]₂ [5], here, we report the synthesis and crystal structure of title compound, P(O)[NHC(O)C₆H₄(2-F)][HNCH(CH₃)₂]₂. This compound appears as two crystallographically independent molecules (A and B) that in each one, the two intermolecular P=O...H—N_{amide} and one C=O...H—N_{C(O)NHP(O)} HBs are responsible to connection of the molecules together as 1-D chains. This result was opposite to that commonly observed for carbacylamido phosphates which show a tendency of phosphoryl group rather than the carbonyl counterpart to form hydrogen bond with the more acidic NH of C(O)NHP(O) skeleton, whereas, the NH of NHR' unit is hydrogen-bonded to C(O). Molecules A and B are very close to each other from a structural point of view. The phosphoryl and carbonyl groups are *anti* to each other and the phosphorus atom has a distorted tetrahedral configuration. The bond angles around the P atom are in the range of 107.11 (8)° to 114.81 (8)°. The P_{amide}-N bond lengths (1.618(6) Å and 1.604(6) Å for A and 1.606(6) Å and 1.612(6) Å for B) are shorter than the P—N_{C(O)NHP(O)} bond (1.705(4) Å for A and 1.698(5) Å for B). The P=O bond lengths (of 1.486(4) Å for A and 1.480(3) Å for B) are standard for phosphoramidate compounds.

Reference:

- [1] Zaburov N. G., Pozdeev O. K., Shamsevaliev F. M., Cherkasov R. A., Gilmanova G. H. (1989) *Pharm. Chem. J.* 23, 423-425.
- [2] Amirkhanov V. M., Orchinnikov V. A., Turon A. V., Skopenko V. V. (1997) *Russ. J. Coord. Chem.*, 23, 126-129.
- [3] Denmark S. E., Fu J., Coe D. M., Su X., Pratt N. E., Griedel B. D. (2006) *J. Org. Chem.*, 71, 1513-1522.
- [4] Tarahhomi A., Pourayoubi M., Rheingold A. L., Golen J. A. (2011) *Struct. Chem.* 22, 201-210.
- [5] Pourayoubi M., Tarahhomi A., Rheingold A. L., Golen J. A. (2010) *Acta Cryst.* E66, o3159.

Synthesis and crystal structure of N-(2-fluorobenzoyl)-N',N'',N'''-tetra(ethyl) phosphoric triamide

A. Tarahhomi^{a,*}, M. Pourayoubi^a

^aDepartment of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran

E-mail: tarahhomi_at@yahoo.com

Carbacylamidophosphates with a C(O)NHP(O) skeleton have attracted attention because of their roles as the O, O'-donor ligands for metal complexation [1]. Following the previous works about carbacylamidophosphates such as preparation of P(O)[NHC(O)C₆H₃(2,6-