

### IRANIAN ORGANIC CHEMISTRY CONFERENCE





## 1\_3 NOV, 2023 UNIVERSITY OF QOM, IRAN

# Synthesis and spectroscopic characterization of a new amidophosphoester, (CH<sub>3</sub>CH<sub>2</sub>O)<sub>2</sub>P(O)NH(C<sub>6</sub>H<sub>10</sub>)NHP(O)(OCH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>

### Narjess Peyman, Mehrdad Pourayoubi\*

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran, nargesspeyman@yahoo.com, pourayoubi@um.ac.ir

Keywords: Amidophosphoester, NMR spectroscopy, Phosphoramide

The phosphoramide compounds have been the focus of researchers for a long time, due to manifold applications, especially in medicine, agriculture, and preparation of flame retardants<sup>[1]</sup>. According to the different applications of these compounds, synthesis methods have been developed, including the reaction of amines with phosphoryl halides<sup>[2]</sup>.

A new amidophosphoester,  $(CH_3CH_2O)_2P(O)NH(C_6H_{10})NHP(O)(OCH_2CH_3)_2$ , was prepared from the reaction of  $(CH_3CH_2O)_2P(O)Cl$  reagent and trans1,4-diaminocyclohexane (2:1 mole ratio, in the presence of  $N(C_2H_5)_3$ ) in dry chloroform (Scheme). The product was characterized by IR,  $^1H$ -NMR,  $^{13}C$ -NMR, and  $^{31}P$ -NMR spectroscopies.

In the IR spectrum, the bands centered at 3201 and 1211 cm<sup>-1</sup> are attributed to the NH and P=O stretching frequencies. The phosphorus signal appears at 8.84 ppm, which is in the range of analogous compound<sup>[3]</sup>. The phosphorus-hydrogen and phosphorus-carbon coupling constants of the title compound are reported.

$$\begin{array}{c|c}
\bullet \\
\hline
P-O \\
\hline
CI
\end{array}$$

$$+ \\
H_2N$$

$$\begin{array}{c}
NH_2 \\
\hline
Chloroform \\
TEA
\end{array}$$

$$\begin{array}{c}
\bullet \\
HN
\end{array}$$

$$\begin{array}{c}
\bullet \\
O-P=O \\
\hline
O\end{array}$$

**Scheme:** Synthesis route of tetraethyl cyclohexane-1,4-diylbis(phosphoramidate).

#### References

- [1] Moghaddam, S. N.; Shabari, A. R.; Sabbaghi, F.; Pourayoubi, M. Synthesis, spectroscopic characterization, crystal structure and Hirshfeld surface analysis of (4-Cl-C<sub>6</sub>H<sub>4</sub>O)(OC<sub>4</sub>H<sub>8</sub>N)<sub>2</sub>PO amidophosphoester. *Rev. Roum. Chim.* 2019, *64* (3), 209–215.
- [2] Bouchareb, F.; Berredjem, M. Recent progress in the synthesis of phosphoramidate and phosphonamide derivatives: A review. *Phosphorus, Sulfur, and Silicon and the Related Elements* 2022, 197 (7), 711–731.
- [3] Handoko.; Benslimane, Z.; Arora, P. S. Diselenide-mediated catalytic functionalization of hydrophosphoryl compounds. *Org. Lett.* 2020, *22* (15), 5811–5816.