ISSN 1070-3632, Russian Journal of General Chemistry, 2006, Vol. 76, No. 8, p. 1344. © Pleiades Publishing, Inc., 2006.
Original Russian Text © M.Zh. Ovakimyan, A.S. Pogosyan, N.M. Kikoyan, M.G. Indzhikyan, 2006, published in Zhurnal Obshchei Khimii, 2006, Vol. 76, No. 8, p. 1400.

LETTERS TO THE EDITOR

Structural Isomerism of Diphenylphosphoryl-2-hydroxyethane

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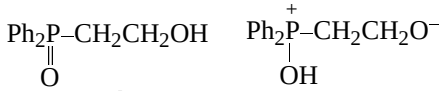
Received October 27, 2005

DOI: 10.1134/S1070363206080366

We found that diphenylphosphoryl-2-hydroxyethane prepared by base hydrolysis of triphenyl-2-hydroxyethylphosphonium chloride [1], according to ^{1}H, ^{31}P, and ^{13}C NMR and mass spectra, is a mixture of two isomeric compounds in 1:3 ratio.

The ^{1}H NMR spectrum taken in $CDCl_3$ contains two multiplets characteristic of PCH_2 and OCH_2 groups, and its ^{13}C NMR spectrum contains two doublets of PCH_2 and two singlets of OCH_2 groups. In the ^{1}H NMR spectrum recorded in DMSO, the OH proton is manifested as a separate signal. Its integral intensity shows that it belongs to the minor product. For more exact assignment of these signals, the correlation between the ^{1}H and ^{13}C NMR spectra was carried out. The ^{31}P NMR spectrum contains two signals in the range characteristic of phosphonium salts: at 34.90 and 30.10 ppm. The molecular ion peak in the mass spectrum is observed at *m/z* 246. Note that the compound under study was also obtained by the similar procedure in [2].

Heating the compound in benzene or toluene for 6–8 h in the absence as well as in the presence of an alkali decreases the yield of the major product. The ^{1}H NMR spectrum shows that the isomer ratio becomes 1:2. Chlorination of the product studied with $POCl_3$ according to [3] gives diphenylphosphoryl-2-chloroethane in a high yield.



A **B**

The data obtained allow a conclusion that the product under study exists as a mixture of the minor form **A** and major form **B**. Existence of the third isomeric form with a five-coordinate phosphorus atom is disapproved by the ^{1}H NMR and ^{31}P NMR data. Identification of the major product as form **B** was based on the higher coupling constant and the lower chemical shift of PCH_2 carbon signal.

^{1}H NMR spectra of $CDCl_3$ and DMSO-d_6 solutions, ^{31}P NMR spectra of $CDCl_3$ solutions, and ^{13}C NMR spectra of $CDCl_3$ solutions were taken on a Varian Mercury-300 (300 MHz) spectrometer. The mass spectrum was recorded on an MKh-1321A device.

REFERENCES

1. Aksnes, G., *Acta Chem. Scand.,* 1961, vol. 15, no. 2, p. 438.
2. Bondarenko, N.A., Matrosov, E.I., Tsvetkov, E.N., and Kabachnik, M.I., *Izv. Akad. Nauk SSSR, Ser. Khim.,* 1980, no. 1, p. 106.
3. Bondarenko, N.A. and Tsvetkov, E.N., *Zh. Obshch. Khim.,* 1989, vol. 59, no. 7, p. 1533.