Phosphorus chemical shifts in some new phosphoramides

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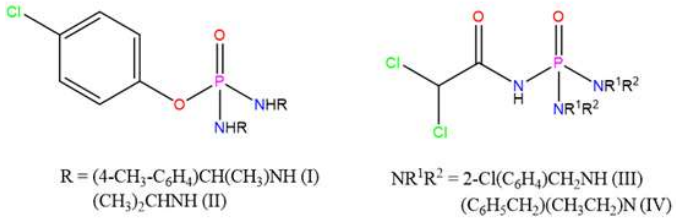
Nuclear Magnetic Resonance (NMR) spectroscopy is an effective tool for identifying compounds and investigating their molecular structures. This technique provide information about the number of equivalent and non-equivalent neighbors to an atom under investigation, the types of functional groups each that nucleus is associated with, and dynamic information. Chemical shift, due to the change in the resonance frequency of the nucleus in different electronic environments, is a valuable tool for detecting changes arising from chemical reactions and geometric isomerism. Extensive databases of chemical shifts allow to predict shifts of target molecules [1,2]. In this study, several new compounds were synthesized and fully characterized using IR, ^{1}H-NMR, ^{13}C-NMR, and ^{31}P-NMR spectroscopy. The synthesized compounds are (4-Cl-C_6H_4O)(4-CH_3-C_6H_4)$CH(CH_3)NH)_2P(O)$ (I), (4-Cl-C_6H_4O)$((CH_3)_2CHNH)_2P(O)$ (II), $(CHCl_2C(O)NH)$(2-Cl-$C_6H_4CH_2NH)_2P(O)$ (III), and $(CHCl_2C(O)NH)((C_6H_5CH_2)(CH_3CH_2)N)_2P(O)$ (IV). The phosphorus chemical shifts in the ^{31}P-NMR spectra were investigated and compared with analogous compounds, and the effects of amine, amide and phenoxy substituents and anisotropic effect caused by arene rings were evaluated. Some topics related to IR and ^{1}H-NMR and ^{13}C-NMR spectra were detailed.



Scheme 1: Chemical structures of compounds (I), (II), (III), and (IV).

References

[1] Jameson, C.J. Understanding NMR chemical shifts. Annual review of physical chemistry 1996, 47, 135–169.
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