NMR parameters of a new phosphoric triamide: N-2,2-dichloroacetyl-N',N''-(bis(isobutyl)phosphoric triamide

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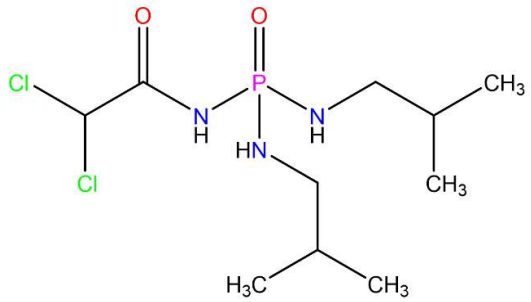
The NMR coupling constants provide information about the different parts of a compound, leading to the assignment of signals, determination of formula[1], conformation, stereochemistry and the nature of chemical bonds[2]. Here, the synthesis of a new phosphoric triamide, $(CHCl_2C(O)NH)((CH_3)_2CHCH_2NH)_2P(O)$, is reported (Scheme 1). In the $^{13}C\{^1H\}$ NMR spectrum, the doublets at 67.32 ppm (J = 11.0 Hz) and 29.89 ppm (J = 5.6 Hz) correspond to the carbon atoms with three-bond separation from phosphorus in amide and amine moieties, respectively. In the ^1H NMR spectrum, a singlet at 9.48 ppm and a doublet of triplet at 4.51 ppm (J = 11.3 and 7.0 Hz) correspond to the NH units of the amide and amine segments, respectively. The two methyl groups of isobutyl segment appear two doublets at 0.84 ppm ($^3J_{HH}$ = 6.6 Hz) and 0.83 ppm ($^3J_{HH}$ = 6.9 Hz). Phosphorus signal in the $^{31}P\{^1H\}$ NMR spectrum is revealed as a singlet at 7.60 ppm.



Scheme 1: Chemical structure of $(CHCl_2C(O)NH)((CH_3)_2CHCH_2NH)_2P(O)$.

References

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