^{1}H and ^{13}C-NMR Spectroscopic Study of Some 1*H*-4,5-Dihydroimidazolium Salts

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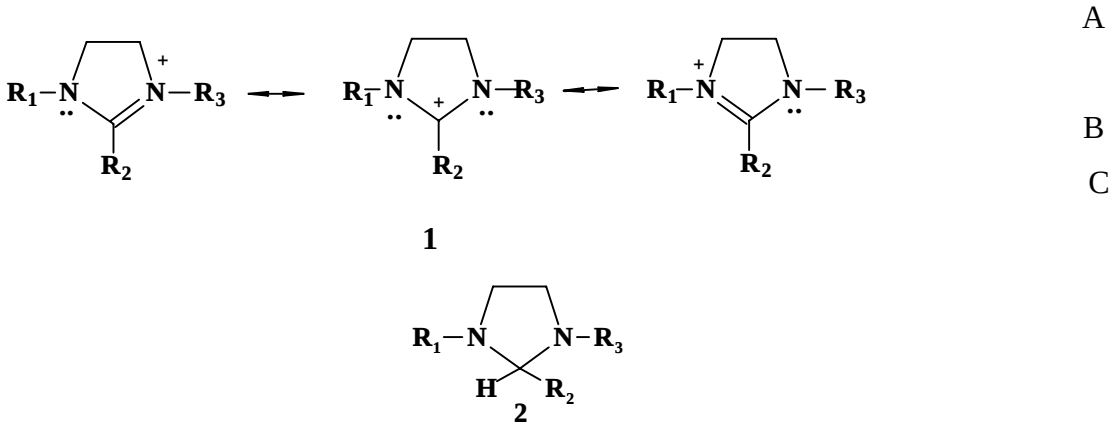
Abstract: The ^{1}H y ^{13}C-NMR spectra of some 1,3 and 1,2,3-trisubstituted 1*H*-4,5-dihydroimidazolium salts are analyzed.

Introduction

1*H*-4,5-Dihydroimidazolium salts are typical cyclic amidinium compounds where the cation is resonance stabilized and the positive charge can be delocalized either on the nitrogen atoms or on the C_2:



NMR spectra analysis and its comparison with the corresponding saturated compounds (imidazolidines 2), allows to reach conclusions about the contribution of such structures.

Experimental

^{1}H and ^{13}C NMR spectra were recorded on a Bruker MSL-300 spectrometer using deuterochloroform as the solvent.

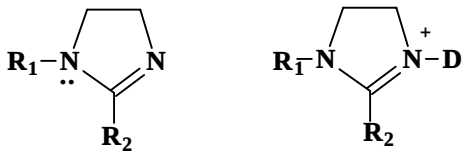
Results and Discussion

The ^{1}H and ^{13}C-NMR spectroscopic study of a series of 1,3-di and 1,2,3-trisubstituted 1*H*-4,5-dihydroimidazoliom salts **1** (Table) is presented.

Table 1.

R_1	R_2	R_3	X^-
C_6H_5	H	C_6H_5	Cl^-
p-$CH_3C_6H_4$	H	*p*-$CH_3C_6H_4$	Cl^-
p-Cl-C_6H_4	H	CH_2-C_6H_5	Cl^-
C_6H_5	C_6H_5	CH_3	I^-
p-$CH_3C_6H_4$	C_6H_5	CH_3	I^-
p-$CH_3OC_6H_4$	C_6H_5	CH_3	I^-
p-$NO_2C_6H_4$	C_6H_5	CH_3	I^-

In order to assign the heterocyclic hydrogens and carbons in the 1,2-diaryl-3-methyl substituted compounds, the spectroscopic study of the parent 1*H*-4,5-dihydroimidazoles **3** and their salts **4** had been carried out.



3 **4**

The unequivocal assignment of the hydrogen and carbon signals of the 1,2,3-trisubstituted salts has been done by the HMQC and HMBC spectra.

The important electronic deficit at the level of the heterocyclic ring in compounds **1** has been clearly demonstrated by comparison of the spectroscopic features of the salts **1** with the corresponding imidazolidines **2**. The iminium structure contribution (A,C) was analyzed according to the chemical shifts and the heteronuclear $^{1}J^{13}C$-H coupling constants of the heterocyclic ring carbons and N-CH_3.