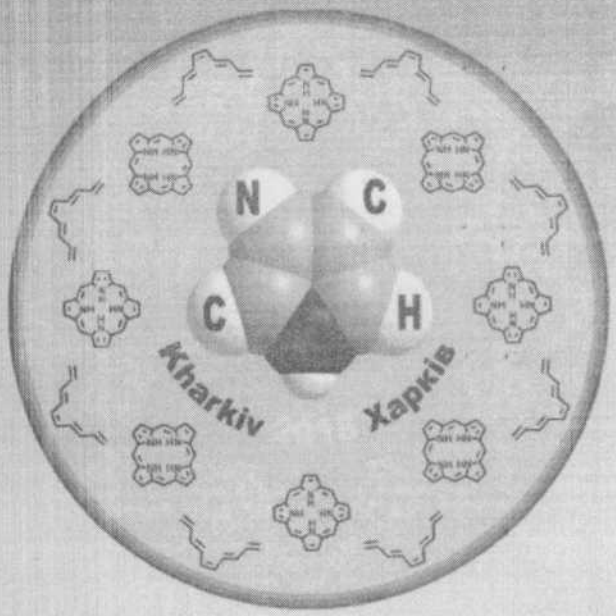
8th International Conference

"CHEMISTRY OF NITROGEN CONTAINING HETEROCYCLES"

in memoriam of Prof. Valeriy Orlov



CNCH-2018

12-16 November, 2018

Kharkiv, Ukraine

Book of Abstracts

ETHYL N-ISOPROPYLOXY-N-1-(4-DIMETHYLAMINOPYRIDINIUM)CARBAMATE CHLORIDE AS A NEW KIND OF ANOMERIC AMIDES

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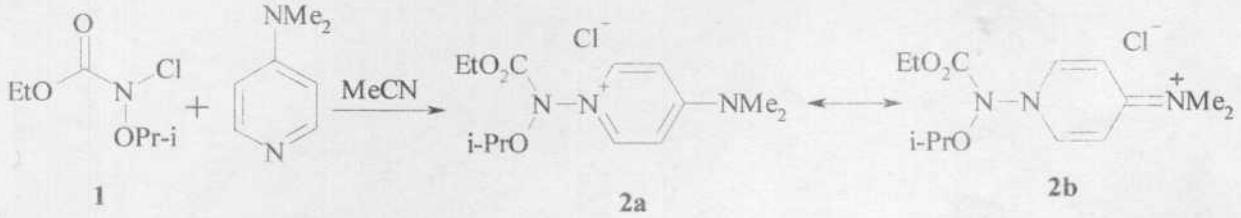
It was found that ethyl N-chloro-N-isopropyloxycarbamate **1** reacted with 4-N,N-dimethylaminopyridine in MeCN yielding relatively stable ethyl N-isopropyloxy-N-1-(4-dimethylaminopyridinium)carbamate chloride **2**, first N-alkoxy-(1-pyridinium)carbamate.



1 **2a** **2b**

Because the structure of received compound was proved also by XRD-study, some interest facts were established: in independent part of the unit cell of crystal of compound **2** there were two organic cations, two Cl^- anions and two molecules of water. In both forms the amide's nitrogen atom has strong pyramidal configuration – the sum of bond angles is 335.6°(in the first form), 335.4°(in the second form).

In compound **2** the $N-N^+$ bond (1.418 Å (in the first form), 1.421 Å (in the second form)) is elongated in compare to the N−N bond in hydrazides of carboxylic acids (1.400 Å). Probably, this $N-N^+$ bond elongation has been caused by $n_{O(Pr\text{-}i)} \rightarrow \sigma^*_{N\text{-}N+}$ anomeric effect action. Amide N−C bond in compound **2** is elongated (1.428 Å (in the first form), 1.419 Å (in the second form)) compare to that in amides (1.359 Å). Lone pair of the central nitrogen atom of system $O\text{-}N\text{-}N^+$ lies in the plane of pyridine ring (the proper torsion angle is -10.4° (in the first form), 14.6° (in the second form). The quinonoid deformation of pyridine ring (structure **2b**) takes place and the positive charge is localized mainly on nitrogen atom of Me_2N-group.