Diffraction Study of Recyclization of Oxazolopyridinium Salts to Indolizines

<u>Dmitry V. Albov</u>, V.B. Rybakov, E.V.Babaev, V.V.Chernyshev, L.A.Aslanov, *Department of Chemistry, Moscow State University, Moscow, Russia*. E-mail: albov@struct.chem.msu.ru

In the course of our systematic study of structure/reactivity relationships for heterocycles, the reaction of recyclization of oxazolo[3,2-a]pyridinium salts with annelated cycloalkane fragments of different size revealed some unexpected peculiarities. All obtained compounds were studied by single crystal (1a-d, 3c, 4b,c) or powder (4d) diffraction. The previous results are reported in [1].

$$R = (CH_2)_n \quad Ar = p - CIPh \quad \frac{|a|b|c|d}{|n|1|2|3|4}$$

$$R = \begin{pmatrix} CH_3 \\ CH_3 \end{pmatrix} \quad CH_3 \quad CH_3$$

$$CIO_4 \quad Ar \quad Ar \quad Ar \quad Ar \quad Ar \quad Aa - d$$

$$R = \begin{pmatrix} CH_3 \\ CH_3 \\ CH_3 \\ Ar \quad Ar \quad Ar \quad Ar \quad Ar \quad Ar \quad Aa - d$$

As discovered earlier, compounds **1b,d** easily gave corresponding indolizines **4b,d**. In the case of compound **1c** the reaction suddenly stopped at the non-predicted intermediate **3c** (with ClO₄ anion). It can be explained by the less distortion of 7-membered ring connected to a non-planar bicycle than in **4c**. Dehydratation of **3c** led to **4c**. Compound **1a** was also attacked by piperidine, but only resin was formed. In this case, the unstable intermediate **2a** is unable to react further because compounds **3a** and **4a** have high angle distortions as the AM1 molecular model shows.

[1] Acta Cryst., 2004, E60, o1096-o1097, o1301-o1302, o2313-o2314. Keywords: structure/reactivity relationship, organic chemistry, powder diffraction