

## Thermal properties of 1-iodomethyl-1,2-dihydro[1,3]-thiasolo[3,2-*a*]quinolinium polyiodides

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Fundamental interest to polyiodide compounds is based on their electronic structure features and the diversity of structural types. Thermal properties of molecular and charge-transfer iodine complexes with various heterocyclic ligands has already been investigated since 1970s according to their perspective properties as organic metals [1]. Though organic polyiodides based on different interactions can also perform various structural transformations, it is still a less studied field. The scope of the present investigation was focused on thermal properties of 2-allylthioquinoline halogenocyclization products.

It is worth noticing that at least three types of organic cations can form various polyiodides in solid state and each group has its own preferences to form I...I, I...H, I...C or I...S interactions. 1-iodinemethyl-1,2-dihydro[1,3]thiasolo[3,2-*a*]quinolinium polyiodides can be included into the group of aromatic heterocycles, in which I...I contacts can be observed as well as I...H, but also short contacts I...C and I...S types can also take place. [2].

Some powder and single crystal 2-allylthioquinoline halogenocyclization products has been synthesised [3]. Their thermal properties will be determined by possible decyclization, loosening of iodine from polyiodide-anion or from CH<sub>2</sub>-I-fragment, elimination of alkyl-radical from thioquinoline or even destruction of heterocyclic system. All this various processes will depend on iodine-cation (I...H, I...C) and I...I interactions in polyiodide-anion.

A thermal analysis of 1-iodinemethyl-1,2-dihydro[1,3]thiasolo[3,2-*a*]quinolinium mono- and polyiodides was performed to make clear the direction of structural transformations. Thermal measurements were carried out in the range 313-573 K with different heating rates in the flow of air. As a result TG, DTG and DTA curves were built. Reaction products in gas phase were studied according to FTIR and mass-spectrometer data.

It was shown that all structural transformations start after the melting point. Among the thermolysis products I-propene, atomic iodine and propene were registered. The ratio of this products in mono- and single crystal triiodide show that in the first case iodine goes away only from -CH<sub>2</sub>-I-fragment and in the second case this process is accompanied by iodine mass loss from the polyiodide anion.

Simultaneous existence of iodopropene with  $m/z=168$  and propene with  $m/z=42$  forms the idea of 2 types of thermal transformations in investigated structures. The first path is to lose proton with the help of iodide-anion, which then makes possible to form  $m/z=42$  particle. The second path is to eliminate iodopropene fragment and formed thioquinolinium cation is stabilized by iodide-anion. It is obvious that both this variants can not be realized in monomolecular reactions, so some molecules follow the first path of transformation while the others – the second. This process was simulated according to quantum-chemical calculations.

[1] R.A. Singh. Bull. Chem. Soc. Jpn, V. 64 (1991) 1938–1943.

- [2] Cambridge Structural Database. Version 5.31. University of Cambridge, UK..
- [3] D.G. Kim. Chemistry of heterocyclic compounds, 11 (2008) 1664-1668.

**1) Poster presentation**