

## **Thermal properties of organic polyiodides with N-alkyl-urotropinium cation**

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Previously was known about thermal properties of charge transfer and molecular complexes of iodine with different organic compounds, including carbohydrates, phenothiazine and fulvalene derivatives [1-2]. These complexes just lose bounded iodine without structural rearrangement while heating. Thermal properties of organic polyiodides are less studied, although they can show wide spectrum of thermal phenomena according to three reasons. The first is vast variety of structural types formed with mono-, triiodide-anions and molecular iodine, which can form 3d-grids and chains [3]. The second one is a diversity of organic cations, capable to form crystalline polyiodides with different intra- and intermolecular interactions. And the last one is a possible thermal structural transformation of organic cation determined by cation–polyiodide binding.

Among many types of found organic cations (quaternary alkyl-ammonium salts, bicyclic and heterocyclic cations), N-alkylurotropinium polyiodides with different anion structures are widely spread in crystallographic databases and can be applied as a useful model to study its thermal properties [4].

A thermal simulation of synthesised crystal and powder samples of N-alkylurotropinium polyiodides using TG, DTG and DTA techniques was made. All thermal investigations were carried out in the range of temperature 313–673 K at a heating rate 1-10 K/min. Thermolysis products in gas phase were registered and identified with Mass- and FTIR-spectrometer data.

Temperature ranges of iodine mass loss were registered. The influence of organic cation structure was studied in saturated (ethyl-) and unsaturated (allyl-) N-alkylurotropinium derivatives. The influence of anion was identified by replacement of iodine to bromine in N-allylurotropinium monoiodide.

A kinetic simulation at different heating rates was held. A sequence of thermolysis stages and its products were proposed. These data were combined with quantum-chemical calculations of I...I, I...H intermolecular interactions within the framework of Atoms in Molecules theory [5]. Iodine-binding features according to this analysis were revealed.

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### **1) Poster presentation**