Sustainability of ionic liquids under the influence of chemical and physical agents

Krivoborodov Efrem Georgievich

Annotation

Currently, the use of ionic liquids is recognized as an alternative to the use of traditional solvents. Based on the current literature data, we can talk about a large number of studies aimed at studying aspects of the practical application of ionic liquids in various qualities. However, information about the chemical and physico-chemical properties of many ionic liquids is not available. Ionic liquids are usually classified as safe and inert reagents, but their reactivity is still poorly studied, so it is important to study the stability of ionic liquids under various reaction conditions.

The open literature describes the interaction of ionic liquids with water, bases, and polysaccharides, which is of particular interest for understanding the fundamental property of IL – the ability to interact with these classes of substances. However, there is no information about the reactivity of IL in relation to simple substances. For this reason, elemental sulfur was chosen as one of the objects of research.

The study of the regularities of the interaction of ionic liquids with elemental sulfur is also of some practical interest, since the disclosure of the S_8 cycle is a key stage in many chemical and technological processes, but is associated with significant energy costs.

In this present work, the physico-chemical stability of ionic liquids under the influence of microwave and gamma radiation, the chemical interaction of phosphonium and imidazolium dialkylphosphate-containing ionic liquids with simple substances (for example, the interaction of 3-*n*-butylmethylphosphonium dimethylphosphate and 1,3-dimethylimidazolium dimethylphosphate with elemental sulfur) are studied.

Scientific novelty

The stability of phosphonium and imidazolium ionic liquids under the influence of microwave and gamma radiation is compared.

It was found that ionic liquids are stable when exposed to microwave radiation, and phosphonium ionic liquids are more stable when exposed to gamma radiation compared to imidazolium ionic liquids.

The interaction of 3-*n*-butylmethylphosphonium dimethylphosphate and 1,3-dimethylimidazolium dimethylphosphate with elemental sulfur was studied for the first time.

The possibility of dimethylphosphate-containing ionic liquids interacting with elemental sulfur has been established by quantum chemical calculations.

It is established that the reaction products of 3-*n*-butylmethylphosphonium dimethylphosphate and 1,3-dimethylimidazolium dimethylphosphate with elemental sulfur are (phosphonooxy)oligosulfanide 3-*n*-butylmethylphosphonium and (phosphonooxy)oligosulfanide 1,3-dimethylimidazolium, respectively.

It is established that the interaction of 3-*n*-butylmethylphosphonium and 1,3-dimethylimidazolium dimethylphosphate with elemental sulfur proceeds by the mechanism of nucleophilic attack by the oxygen atom of the dimethylphosphate-containing anion of the ionic liquid on the sulfur cycle.

Theoretical and practical value

It is established that dialkylphosphate-containing ionic liquids can act as nucleophilic agents in reactions with inorganic cyclic compounds.

A scheme for the synthesis of (phosphonooxy)oligosulfanide 3-*n*-butylmethylphosphonium and (phosphonooxy)oligosulfanide 1,3-dimethylimidazolium without the formation of by-products and using safe reagents, characterized by high energy efficiency.

It is established on the example of formaldehyde polymerization that (phosphonooxy)oligosulfanide 1,3-dimethylimidazolium can act as an initiator of polymerization of electron-deficient monomers.

Key points for the thesis presentation:

Phosphonium and imidazolium ionic liquids have a high degree of stability when exposed to microwave radiation.

Phosphonium ionic liquids are more stable when exposed to gamma radiation compared to imidazolium ionic liquids.

Dialkylphosphate-containing ionic liquids react with elemental sulfur.

The reaction products of ionic liquids of 3-*n*-butylmethylphosphonium dimethylphosphate and 1,3-dimethylimidazolium dimethylphosphate with elemental sulfur are (phosphonooxy)oligosulfanide 3-*n*-butylmethylphosphonium and (phosphonooxy)oligosulfanide 1,3-dimethylimidazolium.

The interaction of 3-*n*-butylmethylphosphonium and 1,3-dimethylmidazolium dimethylphosphate with elemental sulfur proceeds by the mechanism of nucleophilic attack by the oxygen atom of the dimethylphosphate-containing anion of the ionic liquid on the sulfur cycle.

(Phosphonooxy)oligosulfanide 1,3-dimethylimidazolium can act as an initiator of formaldehyde polymerization.