

Ion mobility spectrometry of nitrogen-containing heterocyclic compounds and hazardous chemical substances

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Relevance of the study. Ion mobility spectrometry is a modern separation technique for analyzing trace amounts of chemicals. High speed and sensitiveness, portability of detectors, lack of vacuum systems and radioactive ionization source in functional solution of devices, make this method promising for solving a great number of analytical tasks. However, plenty of possible ion-molecular reactions, proceeding under atmosphere pressure in an ionization source, a drift space of ion mobility spectrometer and also insufficiently explored mechanism of ions formation, make a reliable interpretation of spectra more complicated and do not give possibility to distinguish compounds with close meanings of ion mobility. Due to this, it is necessary to conduct the nature of the ion spectrum dependence on the structure of the molecule fragments and the existence of functional groups, to find additional signals which will increase the selectivity of identifying substances with similar structure and chemical properties.

Developed methodological approaches to analysis of ion mobility spectra allow to determine characteristic signals of individual substances and compare them with probable ions structure.

Establishing a regularity and common areas of ion mobility for substances, similar in structure, also makes it possible to detect classes of compounds.

The detection of ion mobility of derivatives of nitrogen-containing heterocyclic compounds (azols) by spectrometry, is of fundamental and practical interest due to the spread of synthetic drugs with a modified chemical formula, which structure is based on a fragment of aromatic or heteroaromatic series and characteristic functional groups.

At present it is necessary to expand the range of emergency chemical hazardous substances (ECHS) which must be controlled both in production and in crowded places. According to the Methodological recommendations adopted by the Centre for Disaster Medicine "Protection" of the Federal medico-biological agency of Ministry of Health, Russian Federation, "organization of medical and sanitary support during terrorist attacks using dangerous chemical and toxic substances" (approved by the Chief State Sanitary Doctor of Russian Federation from 28th December, 2001 №2510/13132-01-34), a list of compounds for analysis was determined.

Due to this, it is relevant to study the dependence of the nature of ion mobility spectrum on the structure of nitrogen-containing heterocyclic compounds and emergency chemical hazardous substances.

Purpose of the study. The purpose of the thesis is to establish the regularities between the nature of ion mobility spectrum and the structure of the researched nitrogen-containing heterocyclic compounds and emergency chemical hazardous substances for their rapid detection.

To achieve this goal it was necessary to solve the following tasks:

1. Development of methodological approaches to analysis of ion mobility spectrum, the determination of distinctive meanings of ion mobility and of the researched compounds.

2. Experimental research of the dependence of the nature of ion mobility spectrum, in particular, the amplitudes of the signals on concentration of substances in the gas phase.

Evaluation of detection limit and operating range of concentration of ECHS.

3. Quantum-chemical calculation of enthalpies of possible reactions ion formation, an analysis of the obtained data and their accordance to the nature of ion mobility spectrum.

4. Development of sampling methodology and determination of detecting conditions in dependence on physic-chemical properties of the compounds under study.

5. Determination of ion mobility meanings of the researched compounds and the choice of use-oriented signals as a part of database in ion mobility spectrometers.

Scientific novelty:

1. Based on spectral characteristics, ion mobility intervals of monocyclic nitrogen-containing compounds and a group of emergency chemical hazardous substances were revealed in order to evaluate the presence of similar functional fragments in structure of molecules. For the most selected compounds such data were not in existence.

2. For the first time, the interpretation method of ion mobility signals, based on calculations of peak areas and changes in their intensity during a single measurement, has been offered. It allows to evaluate the ions' structure formed in the ion source and in the drift chamber of the ion mobility spectrometers under atmosphere pressure and classify them as monomer and oligomer forms.

3. The comparison of the results of the experimentally obtained ion mobility spectra of the researched groups of compounds with theoretical quantum-chemical calculations of the ion formation enthalpies was carried out.

Practical significance of the study.

Methods of sampling selection depended on the physical and chemical properties of researched compounds have been developed, which significantly increase the efficiency of detecting substances using portable ion mobility spectrometers. This fact is confirmed by the acts of practical use of the results of the thesis by the Limited Liability Company "Modus" and Federal State Budgetary Educational Institution of Higher Education "Russian University of Chemical Technology named after D.I. Mendeleev".

The obtained characteristic values of ion mobility of nitrogen-containing heterocyclic compounds and emergency chemical hazardous substances are contained in the database of ion mobility spectrometers “IDD (ion - drift detector) KERBER-T” and automatic stationary gas detector “Segment” (ASG “Segment”) made in Russia, which are used in Ministry of Internal Affairs (MIA), Federal Security Service (FSS) and Federal Customs Service of Russia (FCS).

The applying of this equipment promotes import substitution of complex analytical equipment.

The detection limits were estimated and the operating ranges were established for detecting emergency chemical hazardous substances.

The developed methods of detecting and analysis of ion mobility spectrum of emergency chemical hazardous substances are used when engineering of the complex non-destructive express testing of postal items “Segment-Post” in order to identify potentially dangerous for life and health of recipients of correspondence as a part of the Strategic Academic Leadership Program “Priority-2030”.

Experimental results of the thesis are used during laboratory practical training on the course “Phisico-chemical methods of analysis of biologically active substances for students of Federal State Budgetary Educational Institution of Higher Education “Russian University of Chemical Technology named after D.I. Mendeleev”.

Provisions submitted for defense:

1. Application of the peaks of ion mobility spectra areas calculation results to establish the correspondence between structures and characteristic signals, particularly for dimer and trimer forms.
2. Establishing the dependency of the nature of ion mobility spectrum of nitrogen-containing heterocyclic compounds and emergency chemical hazardous substances on concentration of the substances under study.
3. The nature of ion mobility spectrum-detection limits and operating ranges of detected compounds.
4. Application of quantum-chemical calculations for the enthalpies of reactions during formation of suggested ions for interpreting signals of ion mobility spectra.