Problems of metrological assurance of gas analysis using IR spectroscopy

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Abstract. The survey article presents the results of work on metrological assurance of measurements using IR spectrometers, IR correlation gas analyzers and CRDS instruments. For the successful application of the existing databases in absorption spectroscopy, it is necessary to identify the most accurate data and assign uncertainty to it, based on experimental studies using reference gas mixtures. The properties of the methods that lead to a deterioration in the measurement accuracy were investigated and the ways were suggested to overcome the shortcomings of the measuring methods.

Available spectroscopic databases and catalogs of spectral parameters of gases were collected without the participation of the metrological community. This is the reason why modern spectral optical methods are not fully implemented in gas analysis. However, it is possible to use the available spectroscopic databases for high-precision measurements. In this paper, we present our approach to measuring the concentrations of gas components in gas mixtures using the spectroscopic HITRAN or GEISA databases.

One of the most promising measurement methods with the help of spectral equipment is the use of universal spectral equipment - IR spectrometers, as well as those with sufficiently high technical and metrological characteristics, IR correlation gas analyzers and CRDS instruments for certification of multi-component gas mixtures.

Two conditions are required for reliable determination of concentration using calculated spectra:

1. Accurate knowledge of lines parameters (e.g. GEISA, HITRAN databases).
2. Accurate knowledge of instrument technical parameters (instrument function in particular).

For the successful application of the existing databases in absorption spectroscopy, it is necessary to identify the most accurate data and assign uncertainty to it, based on our own experimental studies using reference gas mixtures. In the future, it will be possible to measure concentration, without the use of reference gas mixtures. To determine the instrument function, it is proposed to use a sealed reference cell with a gas (for example, CO or Hbr). The gas should have relatively narrow lines (or groups of lines) in the absorption spectrum in the IR region. The use of such a cell will allow to fairly accurately

restore the instrument function and to control its stability over time, making the necessary adjustments.

When determining the concentration of gases using the calculation method, it is enough once (using reference gas mixtures) to obtain the correction factors between the actual concentrations and the calculated ones. Further similar measurements can be implemented on another device. The only condition is the use of a reference gas cell to determine the instrument's instrument function [1-3].

In the case of IR correlation spectroscopy, there is investigated the effect of interfering components on the measurement of the component under study and a method of compensation of interference is proposed [4].

In the case of CRD spectroscopy, there have been investigated several effects that eliminate the advantages of the method [5].

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