AUTOMATION OF THE PROCEDURE FOR DETERMINING SPECTRAL LINE HALF–WIDTH AND SHIFT FROM OPTO–ACOUSTIC MEASUREMENTS

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In this paper we propose a technique for automating the procedure for determining the parameters of spectral lines based on search of the initial approximation for the least–square method using spline function. Some results of numerical simulations and data of processing actual line of water vapor recorded with a dual–channel opto–acoustic (OA) laser spectrometer are also presented in the paper.

The study of characteristics of molecular absorption line contour in gases is topical for solving direct and inverse problems of planetary atmosphere optics, remote sounding of gas constituents distribution in the atmosphere, and other problems.

Such parameters of spectral line as half–width (γ), center shift (δ) are determined from high resolution laser spectrometer measurements.[1–8] The experimental data are usually processed by the method of fitting the theoretical model of absorption line contour (this is most commonly the Voigt contour, Refs. 3–7) to the one $\xi(\nu)$ measured using the least–square method (LSM). This method is widely used for such processing but to employ it advantageously one must assign zero approximations of unknown parameters. In our paper we offer to use a smoothing spline for computer determination of zero approximation of the sought absorption line parameters from the experimental data.

The absorption line contour measurement results are smoothed with the help of a spline.[9,10] It is easy to find the maximum value K_m at the line center and the half–width γ at the level of 0.5 K_m from the derived smoothed values.

Let us assume that the smoothed contour can be represented as

$$K_m \Psi(\nu, \gamma) = K_0 F(\nu, \gamma) + \varphi , \qquad (1)$$

where $\Psi(\nu, \gamma)$ is the shape of the smoothed absorption line contour; $F(\nu, \gamma)$ corresponds to the chosen theoretical model of absorption line; K_0 defines the value of the absorption coefficient at the line center ν_0 ; and, φ is some nonselective component of measurements (background) which is usually available in opto–acoustic (OA) measurements.[1,2]

If the approximated value γ obtained using the spline is employed as a line half–width, then the unknown values of K_0 and φ can be easily estimated by the formulas

$$K_0 = K_m \frac{\Psi(\nu_1, \gamma) - \Upsilon(\nu_2, \gamma)}{F(\nu_1, \gamma) - F(\nu_2, \gamma)} , \qquad (2)$$

$$\varphi = K_m \frac{F(\nu_1, \gamma)\, \Psi(\nu_2, \gamma) - F(\nu_2, \gamma)\, \Psi(\nu_1, \gamma)}{F(\nu_1, \gamma) - F(\nu_2, \gamma)} . \qquad (3)$$

Here ν_1 and ν_2 are some frequencies around the line center which must satisfy the conditions $\nu_1, \nu_2 < \nu_0$ or $\nu_1, \nu_2 > \nu_0$.

The found values K_0 , ν_0 , γ, and φ can be used as zero approximation for LSM–fitting of the theoretical model to the experimental results.

The efficiency of our method has been checked using numerical simulation. The quality of the line parameter reconstruction is depicted in Fig. 1, where the reconstruction results of the simulated Voigt line parameters for $\gamma = 0.5$ cm^{-1} at the background level of 10% of the maximum value of the function are presented. The measurement error ε (in per cent of the background level) and contour parameter reconstruction Δ (ν_0 , γ, and φ) errors are plotted on the abscissa and ordinate, respectively. As seen in the figure, the obtained initial approximations, even with substantial noise in the initial data, allow one to determine the sought parameters fairly well.

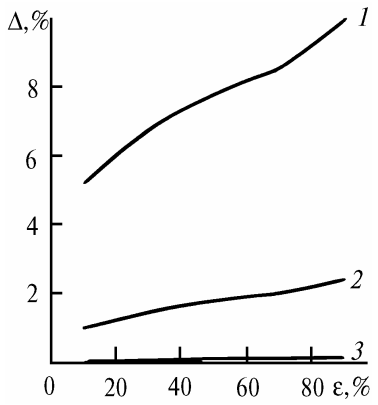

FIG. 1. Results of numerical simulation on reconstructing the absorption line center ν_0 (curve 1), half–width γ (curve 2), and background (curve 3).

To test the method described we processed the measurement results of the H_2O absorption line contours with the center $\nu_0 = 14\,397.364$ cm^{-1} broadened with noble gases He, Ne, Ar, Kr, and Xe. The measurements were made using a dual–channel OA spectrometer. The measurement procedure is described in detail in Refs. 2 and 7. It consists in that two OA cells are positioned successively on the laser beam axis. One of them is filled with pure water vapor at pressure of several torrs and the other with water vapor – buffer gas mixture at pressure $P_{buf} \gg P_{H_2O}$. The measurements in the first OA cell give the Doppler contour of the absorption line

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while those in the second one provide the contour of the same line but broadened with buffer gas pressure.

The measurement results are depicted in Figs. 2*a–e*. A number of laser generation wavelengths N falling into the absorption line contour are plotted on the abscissa, and the OA signal amplitude U in relative units is plotted on the ordinate. The dots denote the experimental data, and a solid line is the contour obtained using the least–square method.

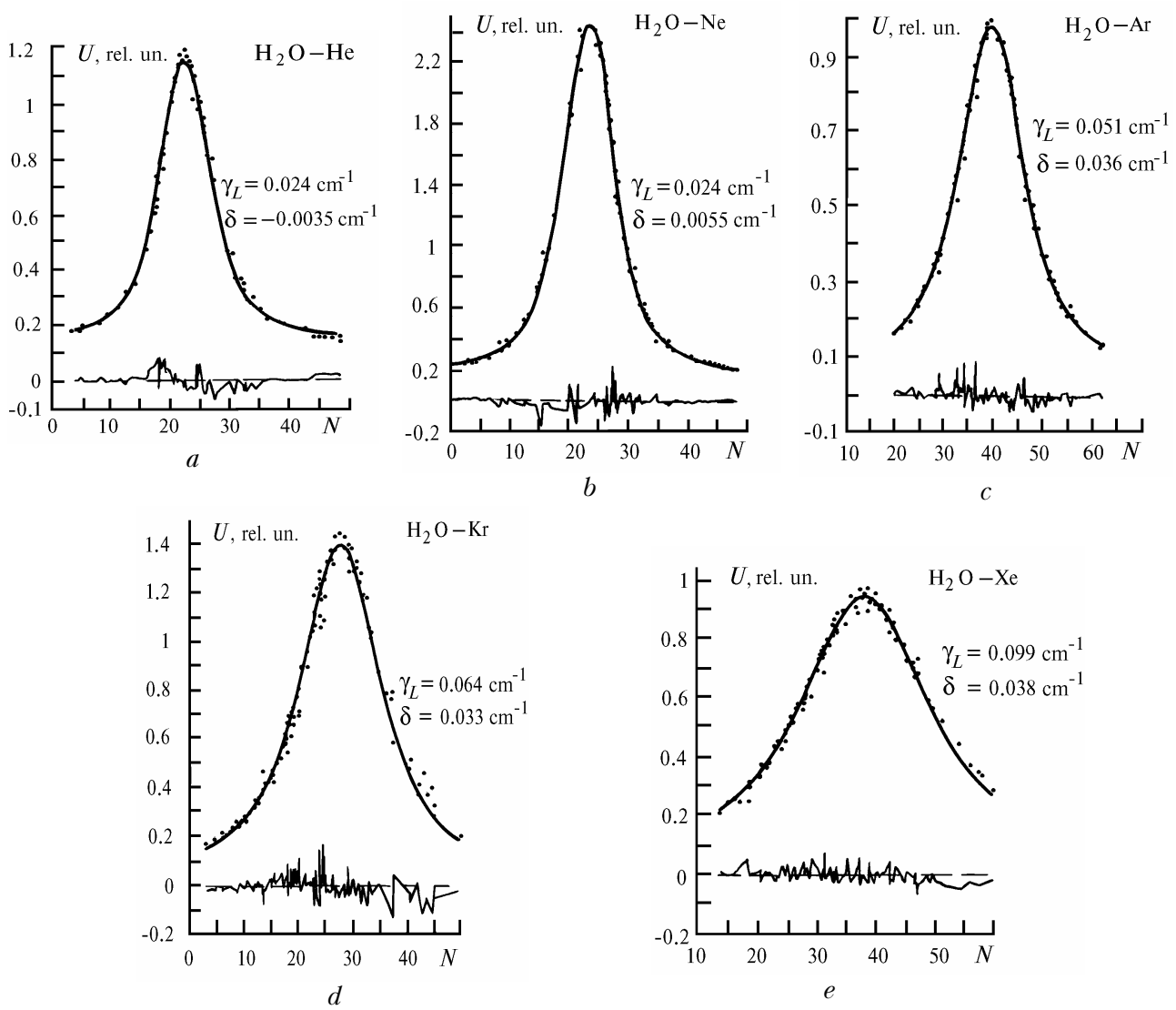

Fig. 2. Experimentally obtained H_2O absorption line contour (dots) broadened with noble gases He *(a),* Ne *(b),* Ar *(c),* Kr *(d), and* Xe *(e), and its processing with the help of LSM (solid line). At the bottom of the figures there is discrepancy between the contour obtained with LSM and the experimental dots.*

In conclusion it should be noted that our fully automated method of processing can be used for automating the determination of the half–width and shift of absorption lines from the OA measurements.

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