# EVALUATION OF EXTINCTION COEFFICIENTS OF $C_{60}$ and $C_{70}$ SOLUTIONS USING PC

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## Introduction

At present arc synthesis of fullerenes is the most accessible and wide-spread method for production of fullerene-containing soot. Percentage of fulerenes in the soot ranges from 6 to 42 wt.%. The fullerene yield strongly depends on many technological parameters: chemical purity of graphite sputtered, its form, geometric dimensions of graphite cores. It is necessary to check the effect that the change of any parameter of synthesis exerts.

Therefore, fullerene percentage in the soot sample is determined. Spectrophotometric analysis is often used for this purpose. The method involves mathematical apparatus wich requires much time for calculations, tables and plots.

We have designed and proposed the computer program to simplify processing spectrophotometric data. This program allows calculation of $C_{60}$ and $C_{70}$ concentrations for short time using values of optical densities and molar extinction coefficients.

## Results and discussion

Using the program designed, the required individual $C_{60}$ and $C_{70}$ concentrations in the solutions of their mixture are determined by solving the system of linear equations:

$$\begin{cases} A_1 = \varepsilon_{60}^1 \cdot X + \varepsilon_{70}^1 \cdot Y \\ A_2 = \varepsilon_{60}^2 \cdot X + \varepsilon_{70}^2 \cdot Y \end{cases} \qquad (1)$$

where $A_1$ and $A_2$ - optical densities of the solution studied for $\lambda_1$ and $\lambda_2$ waves, respectively;

$\varepsilon_{60}^1$ and $\varepsilon_{60}^2$ - molar extinction coefficients of $C_{60}$ solution;

$\varepsilon_{70}^1$ и $\varepsilon_{70}^2$ - molar extinction coefficients of $C_{70}$ solution for $\lambda_1$ and $\lambda_2$ wave lengths, respectively;

X and Y - mole $C_{60}$ and $C_{70}$ concentrations in the solution studied.

From the theoretical and practical viewpoints, ratio of $C_{60}$ and $C_{70}$ concentrations in the fullerene-containing soot is of great importance. In the work presented the ratio is determined by the equation:

$$\frac{X}{Y} = \frac{\varepsilon_{70}^2 - \varepsilon_{70}^1}{\varepsilon_{60}^1 - \varepsilon_{60}^2}, \qquad (2)$$

attained by solving system (1) in the case when $A_1=A_2$. The exact values of molar extinction coefficients for $C_{60}$ and $C_{70}$ solutions are important to diminish the error made in qualitative analysis of fullerene solutions.

The literature data on molar extinction coefficients are ambiguous [1-23]. In the work presented the molar extinction coefficients have been determined using plots $I_{pb}= f(lg\ C)$ (Ringbom curve) [4], where $I_{pb}$ - intensity of the beam passed (in %), C - molar concentration of $C_{60}$ or $C_{70}$. Ringbom curves obtained experimentally for $C_{70}$ toluene solutions are given in Fig.1.

Fig.1 shows plots for $\lambda$=407 nm (1) and $\lambda$=472.8 (2). As seen in Fig.1, the $C_{70}$ concentration range "$\delta_1$" and " $\delta_2$" corresponds to the optical density equals 0.4343 relative units [4] what resulted from the error made in measurements of optical density of $C_{70}$ solutions. Therefore, the values of molar extinction coefficients, obtained graphically, have been checked by the method of mathematical approximations using the computer program designed by authors.

## Conclusions

The designed computer program allows acceleration of processing experimental results in several times and revealing promising directions for investigations.

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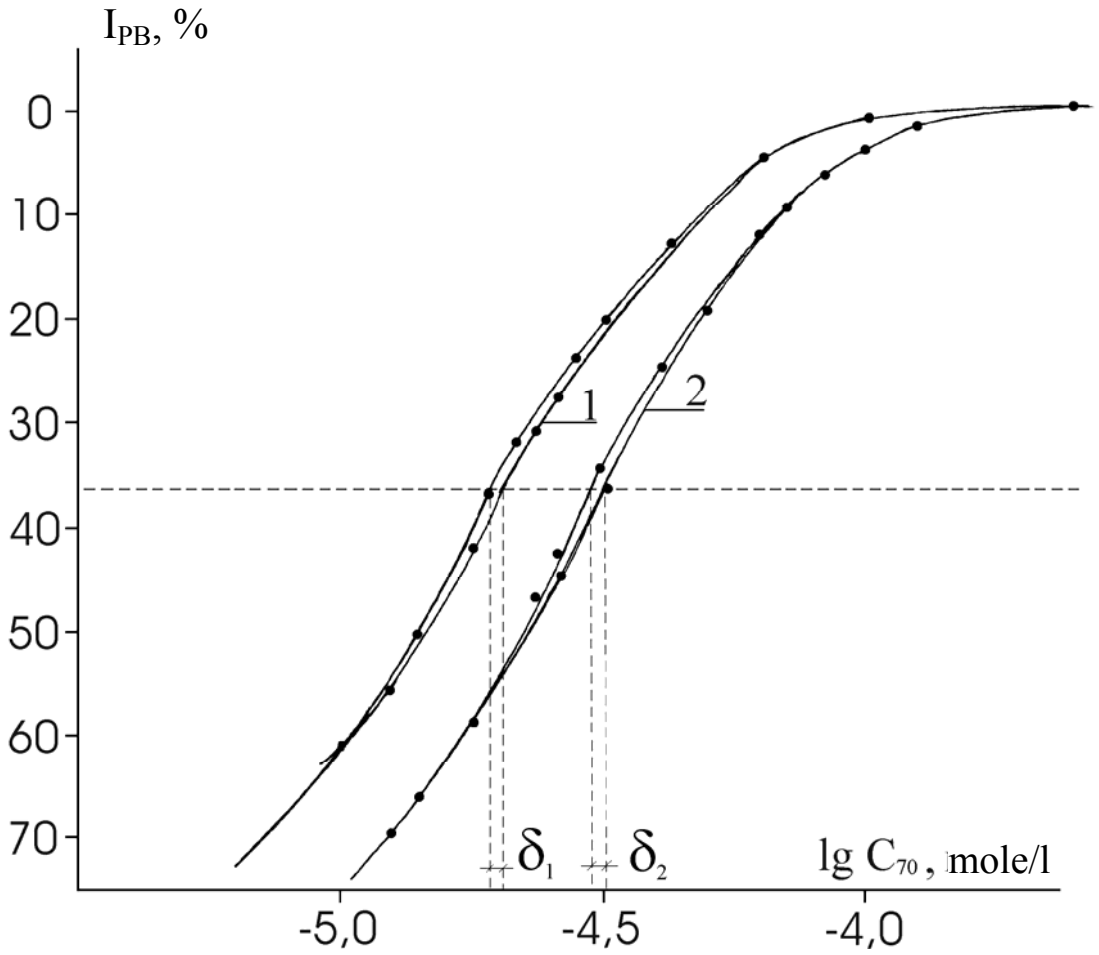


Fig.1. Intensity of the beam passed $I_{pb}$ (in %) vs. logarithm of mole concentration for $C_{70}$ toluene solution for wave lengths: 1 - 407 hn, 2 - 472.8 nm; $\delta_1$ and $\delta_2$ - concentration ranges which used to calculate mole extinction coefficients for $\lambda$=407 nm (1) and $\lambda$=472.8 (2), respectively.