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

Maystrenko M.I.*, Anikina N.S., Zolotarenko A.D., Lysenko E.A., Sivak G.A., Schur D.V.

Institute for Problems of Materials Science of NAS of Ukraine, lab. # 67, 3, Krzhizhanovsky str., Kiev, 03142 Ukraine

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 λ_1 and λ_2 waves, respectively;

ε_{60}^1 and ε_{60}^2 - molar extinction coefficients of C_{60} solution;

ε_{70}^1 и ε_{70}^2 - molar extinction coefficients of C_{70} solution for λ_1 and λ_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 λ=407 nm (1) and λ=472.8 (2). As seen in Fig.1, the C_{70} concentration range "δ_1" and " δ_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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* Fax: (+38) 044-424-0381 E-mail: shurzag@materials.kiev.ua

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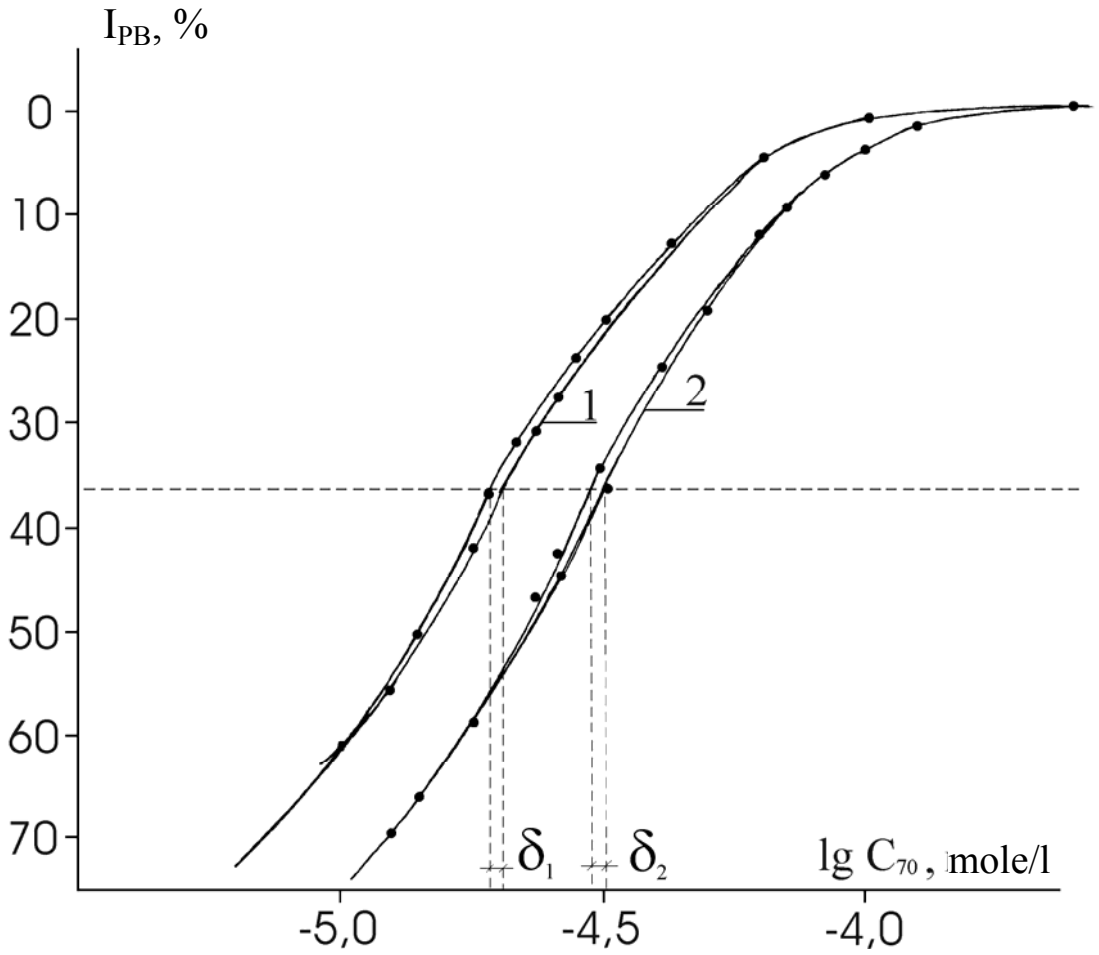

Fig.1. Intensity of the beam passed I_{pb} (in %) vs. logarithm of mole concentration for C_{70} toluene solution for wave lengths: 1 - 407 hn, 2 - 472.8 nm; δ_1 and δ_2 - concentration ranges which used to calculate mole extinction coefficients for λ=407 nm (1) and λ=472.8 (2), respectively.

ОПРЕДЕЛЕНИЕ КОЭФФИЦИЕНТОВ ЭКСТИНКЦИИ РАСТВОРОВ C_{60} И C_{70} С ПОМОЩЬЮ ЭВМ

Майстренко М.И.*, Аникина Н.С., Золотаренко А.Д., Лысенко Е.А., Сивак Г.А., Щур Д.В.

Институт Проблем Материаловедения НАН Украины, Лаборатория №67,
ул. Кржижановского 3, Киев, Украина

Введение

В настоящее время дуговой синтез фуллеренов является самым доступным и распространенным методом получения фуллеренсодержащей сажи. Процентное содержание фуллеренов в ней колеблется от 6 до 24% (мас.). На выход фуллеренов сильное влияние оказывают многие технологические параметры: от химической чистоты испаряемого графита до его формы и геометрических размеров графитовых стержней. Влияние изменения любого из параметров синтеза на выход фуллеренов необходимо отслеживать.

Для этого в пробе сажи определяется процентное содержание фуллеренов. Часто таким методом анализа является спектрофотометрический метод, использующий математический аппарат, который требует значительных затрат времени на выполнение вычислений, составление таблиц и построение графиков.

Для упрощения процесса обработки спектрофотометрических данных нами разработана и предложена компьютерная программа, позволяющая вычислить концентрации C_{60} и C_{70} за короткий срок по введенным значениям оптических плотностей и молярных коэффициентов экстинкции.

Результаты и обсуждение

С использованием разработанной программы необходимые индивидуальные концентрации C_{60} и C_{70} в растворах их смеси определяются путем решения системы линейных уравнений:

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

где A_1 и A_2 – оптические плотности исследуемого раствора для волн λ_1 и λ_2 соответственно;

ε_{60}^1 и ε_{60}^2 – молярные коэффициенты экстинкции раствора C_{60};

ε_{70}^1 и ε_{70}^2 – молярные коэффициенты экстинкции раствора C_{70} для длин волн λ_1 и λ_2, соответственно;

X и Y – мольные концентрации C_{60} и C_{70} в исследуемом растворе.

С теоретической и практической точек зрения важное значение имеет величина отношения концентраций C_{60} и C_{70} в фуллереносодержащей саже, которое, в настоящей работе определялось из уравнения

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

полученного при решении системы (1) в случае, когда $A_1=A_2$. Для уменьшения ошибки при количественном анализе растворов фуллеренов особенно важно иметь точные значения молярных коэффициентов экстинкции растворов C_{60} и C_{70}.

Имеющиеся в литературе значения молярных коэффициентов экстинкции неоднозначны [1, 2].

В настоящей работе молярные коэффициенты экстинкции определяли с использованием графиков $I_{пр}=f(lg\ C)$ (кривых Рингбома) [4], где $I_{пр}$ – интенсивность прошедшего луча (в %), C – молярная концентрация C_{60} или C_{70}. Примеры экспериментально полученных кривых Рингбома для толуольных растворов C_{70} приведены на рис. 1.

Как видно из рисунка, на котором приведены графики для λ=407 нм (1) и λ=472,8 (2), из-за ошибок измерения оптической плотности растворов C_{70}, оптической плотности, равной 0,4343 относительных единиц [4], соответствует интервал концентраций C_{70} "δ_1" и " δ_2". Поэтому,

* Fax: (+38) 044-424-0381 E-mail: shurzag@materials.kiev.ua

полученные графическим путем значения молярных коэффициентов экстинкции уточнялись методом математических приближений с использованием разработанной авторами статьи компьютерной программы.

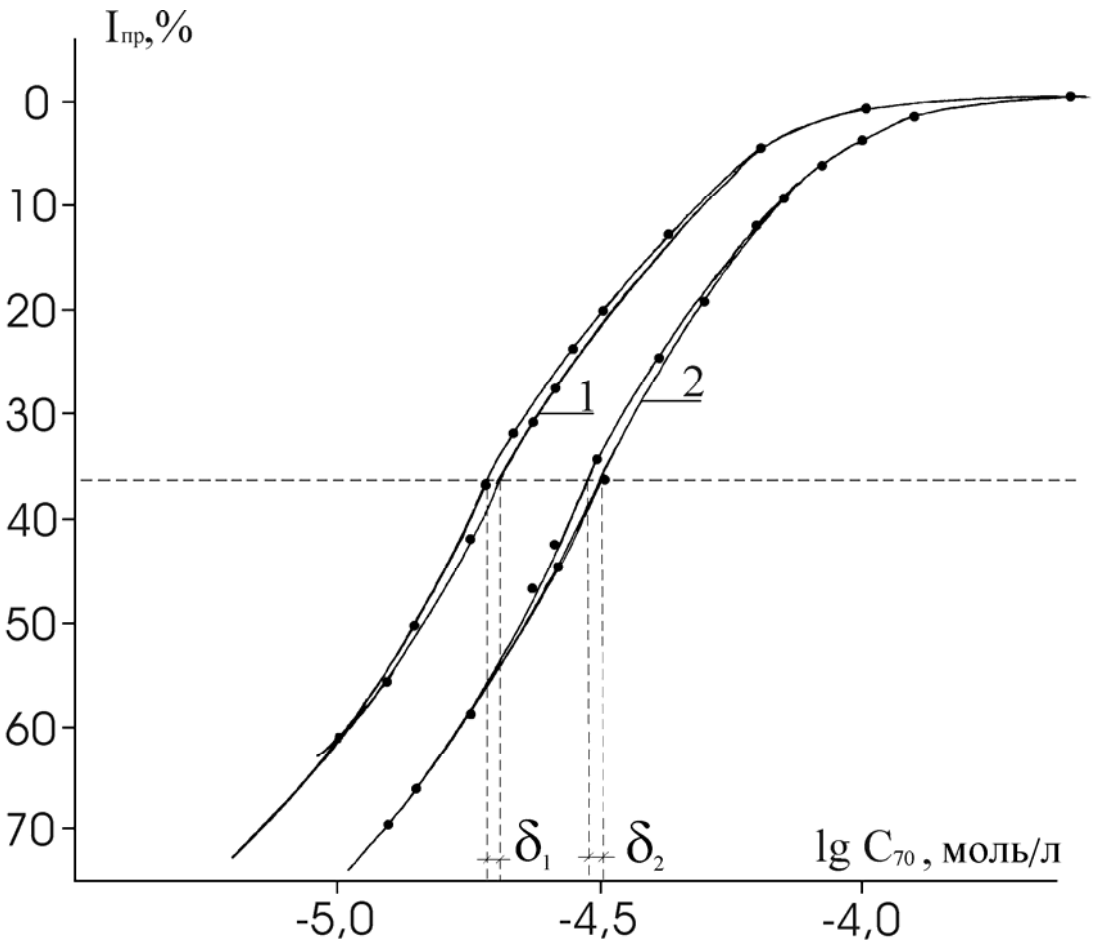

Рис. 1. Зависимость интенсивности прошедшего луча $I_{пр.}$ (в %) от логарифма мольной концентрации толуольного раствора C_{70} для длин волн: 1 – 407 нм, 2 – 472,8 нм; δ_1 и δ_2 – интервалы концентраций, которые использовались при расчетах мольных коэффициентов экстинкции для λ=407 нм (1) и λ=472,8 (2), соответственно.

Выводы

1. Разработана компьютерная программа, позволяющая ускорить обработку результатов эксперимента, а также выявить перспективные направления исследований.
2. Использование разработанной компьютерной программы позволяет в несколько раз ускорить обработку результатов эксперимента.

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