CHEMISTRY AND CHEMICAL ENGINEERING

Volume 2022 | Number 1 Article 8

May 2022

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Recommended Citation

KOZINSKAYA, Lyubov and MIRKHAMITOVA, Dilorom (2022) "MATHEMATICAL MODELING OF SYNTHESIS 4´,4´´-DI-(1-METHYL-1-HYDROXY-2-PHENYLETHYNYL)-DIBENZO-18-CROWN-6," *CHEMISTRY AND CHEMICAL ENGINEERING*: Vol. 2022: No. 1, Article 8.
DOI: 10.34920/cce202218
Available at: https://cce.researchcommons.org/journal/vol2022/iss1/8

MATHEMATICAL MODELING OF SYNTHESIS 4′,4′′-DI-(1-METHYL-1-HYDROXY-2-PHENYLETHYNYL)-DIBENZO-18-CROWN-6

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The main goal of this study is the mathematical modeling of the optimal conditions for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 by the least squares method. In the STAT program, iconograms of mathematical modeling of the synthesis and the dependence of the rate of formation of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 on temperature and reaction time were obtained, the corresponding analytical dependencies are determined. Mathematical processing of the results of the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 was carried out, a system of linear equations was compiled using the matrix method. The average reaction rate and the optimum of the mathematical model were determined, and the experimental and calculated data on the yields of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 were compared.

Keywords: 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6, mathematical model, matrix, least squares method

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ СИНТЕЗА 4′,4′′-ДИ-(1-МЕТИЛ-1-ГИДРОКСИ-2-ФЕНИЛЭТИНИЛ)-ДИБЕНЗО-18-КРАУН-6

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Основной целью данного исследования является математическое моделирование оптимальных условий синтеза 4′,4′′-ди-(1-метил-1-гидрокси-2-фенилэтинил)-дибензо-18-краун-6 методом наименьших квадратов. В программе STAT получены иконограммы математического моделирования синтеза и зависимости скорости образования 4′,4′′-ди-(1-метил-1-гидрокси-2-фенилэтинил)-дибензо-18-краун-6 от температуры и продолжительности реакции, определены соответствующие аналитические зависимости. Проведена математическая обработка результатов синтеза 4′,4′′-ди-(1-метил-1-гидрокси-2-фенилэтинил)-дибензо-18-краун-6, составлена система линейных уравнений матричным способом. Определены средняя скорость реакции, оптимум математической модели, сопоставлены экспериментальные и расчетные данные выходов 4′,4′′-ди-(1-метил-1-гидрокси-2-фенилэтинил)-дибензо-18-краун-6.

Ключевые слова: 4′,4′′-ди-(1-метил-1-гидрокси-2-фенилэтинил)-дибензо-18-краун-6, математическая модель, матрица, метод наименьших квадратов

4′,4′′- DI-(1-METIL-1-GIDROKSI-2-FENILETINIL)-DIBENZO-18-KRAUN-6 SINTEZINI MATEMATIK MODELLASHTIRISH

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Ushbu tadqiqotning asosiy maqsadi kichik kvadratlar usuli bilan 4′,4′′-di-(1-metil-1-gidroksi-2-feniletinil)-dibenzo-18-kraun-6 sintezining maqbul sharoitlarini matematik modellashtirishdir. STAT dasturida 4′,4′′-di-(1-metil-1-gidroksi-2-feniletinil)-dibenzo-18-kraun-6 hosil bo'lishiga reaksiya tezligi, harorati va vaqt davomiyligini analitik bog'liqligi aniqlanib matematik modellashtish ikonogrammalari olindi. 4′,4′′-Di-(1-metil-1-gidroksi-2-feniletinil)-dibenzo-18-kraun-6 sintez natijalari matematik qayta ishlash amalga oshirildi, matritsa usulida, chiziqli tenglamalar tizimi tuzildi. Reaktsiyaning o'rtacha tezligi, matematik modelning optimalligi aniqlandi, 4′,4′′-di-(1-metil-1-gidroksi-2-feniletinil)-dibenzo-18-kraun-6 unumlarining eksperimental va hisoblangan ma'lumotlari taqqoslandi.

Kalit so'zlar: 4′,4′′-di-(1-metil-1-gidroksi-2-feniletinil)-dibenzo-18-kraun-6, matematik model, matritsa, kichik kvadratlar usuli

DOI: 10.34920/cce202218

Introduction

Molecules containing hydroxyl groups and fragments of multiple carbon-carbon bonds are often found in nature. For example, the ground part of lower [1] and higher plants [2], as well as a component of algae [3] and sea anemones [4] in aquatic environments. Molecules of acetylenic alcohols [5] are active at several reaction centers [6, 7], have the ability to form hydrogen bonds [8, 9], many of them have antimicrobial [10] and other properties [11]. Acetylene lipids have been created to determine the configurations of aminoalkanes [12] and many others [13]. Lipid alkynylcarbinols constitute a class of potential antitumor compounds [14].

The introduction of an ethynylcarbonyl fragment leads to an increase in analgesic properties and a decrease in toxicity [15].

Traditional planning and implementation of syntheses [16] based on knowledge of the basic mechanisms of chemical reactions do not meet modern requirements in terms of the amount of reagents [17], solvents [18], and reaction time [19]. Mathematical modeling makes it possible to take into account the largest number of factors and phenomena that affect the course of real chemical processes [20].

Mathematical modeling provides high accuracy in predicting the results of experiments on calculations [21]. As a result, the number of experiments that had to be carried out earlier to ensure reliable reproducibility of the experiment [22], the study of such factors as temperature[23], pressure [24], solvent nature [25], reaction time, etc., can be significantly reduced [19]. This leads to the required economic, experimental, energy and ma-

terial indicators of modern processes [26]. If necessary, these models can be supplemented with the required new relationships, which leads to more accurate quantitative results [27].

Research methods

The article presents the calculation of a mathematical model for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 by the least squares method.

Using the STAT computer simulation program, iconograms of the dependence of the reaction rate on temperature and process time are shown.

The matrix method shows the system of linear equations of analytical dependences of the optimal conditions for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6.

Results and discussions

Mathematical calculation of the study of the kinetic parameters of chemical reactions allows us to conclude that it is in principle possible to interact 4′,4′′-diacetyldibenzo-18-crown-6 with phenylacetylene according to the Favorsky reaction [28] to obtain 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 under certain conditions, with given parameters, as well as the possibility of calculating the depth of this chemical transformation [29].

With a detailed analysis of the mathematical model of the interaction of the initial substances of a chemical reaction, it is possible to control the kinetic parameters of the process [30].

Mathematical modeling of the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 by the Favorsky reaction using the STAT program was carried out. The objective functions in mathematical modeling were the quantitative yield and the rate of formation of the main product. The working functions were given the reaction time - the duration of the presence of substances in one volume, and the reaction temperature.

On the iconogram of the mathematical model for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 (Fig. 1, 2), the temperature and duration of the reaction have an "extreme" character:

The range of the reaction time is given taking into account the literature data and is 3 hours.

The dependence of the yield of the target product w(y) on the temperature t and the reaction time has the form:

$$w = -122,23 + 3,04x_1 - 0,017x_1^2 + \\ + 1,67\,x_2 - 0,36x_2^2 \quad (1)$$

where: w - yield of 4',4''-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 (%); x_1 - temperature (°C); x_2 – reaction time (hour).

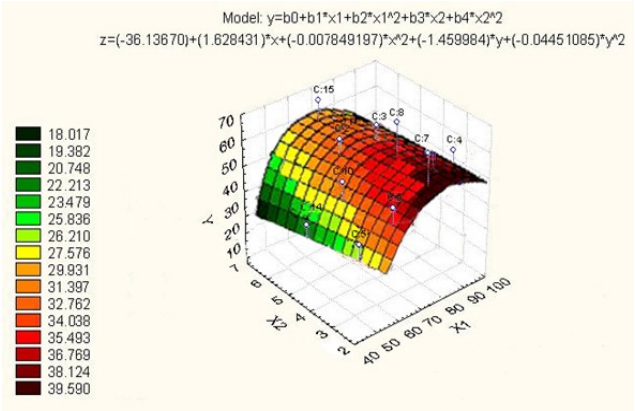


Figure1. Iconogram of mathematical modeling of the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6.

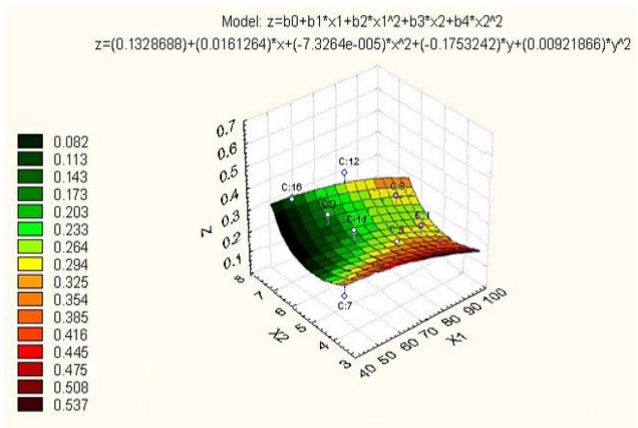
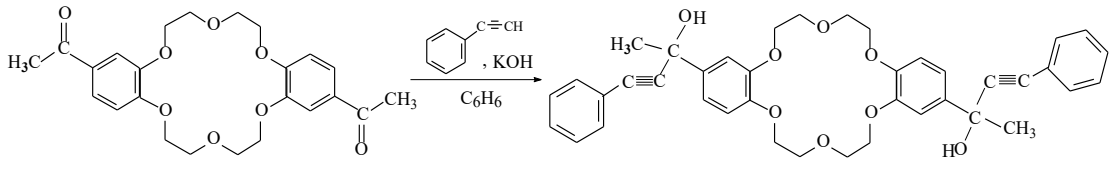


Figure 2. Iconogram of the dependence of the reaction rate of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 on temperature and reaction time.



The STAT program was used to simulate the reaction rate of the formation of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 depending on the temperature and reaction time:

$$z = -17{,}19 + 0{,}68x_1 - 0{,}0041x_1^2 + 3{,}76\,x_2 + 0{,}53\,x_2^2 \quad (2)$$

where: z- rate of formation of 4′,4′′-di-(1-methyl-1-hydroxyethynyl)-dibenzo-18-crown-6 (mol/l·s·10-3); x_1 – temperature (°C); x_2 – reaction time, residence time of substances in the reactor (hour).

The technological criterion for optimizing the conditions for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 was taken as the maximum yield:

$$w(x_1, x_2) \rightarrow max \quad (3)$$

The optimum of the mathematical model is achieved at a fixed output of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 has the form:

$$w = b_0 + b_1x_1 + b_2x_1^2 + b_3x_2 + b_4x_2^2 \quad (4)$$

differentiating the "w" of this equation with respect to each of the variables x_1 and x_2 we obtain:

$$\begin{cases} \frac{\partial w}{\partial x_1} = b_1 + 2b_2x_1 = 0 \\ \frac{\partial w}{\partial x_2} = b_3 + 2b_4x_2 = 0 \end{cases} \quad (5)$$

When solving the system of equations, we find the values x_1 and x_2:

$$x_1 = -\frac{b_1}{2b_2} \quad \text{and} \quad x_2 = -\frac{b_3}{2b_4} \quad (6)$$

When substituting the found values of the coefficients b_1, b_2, b_3 and b_4 from equations (1-6), we find the optimum points x_1 and x_2:

$x_1 = 76{,}8$ °C; $x_2 = 2{,}96$ hour, w = 68,7%;
$z = 2{,}48 \cdot 10^{-4}$ mol/l·h.

Mathematical processing of synthesis results 4',4''-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6

Table 1

Dependence of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 on the reaction temperature

t_1	20	30	40	50	60	70	80	90	100
y_1	14	20	32	47	54	62	70	65	64

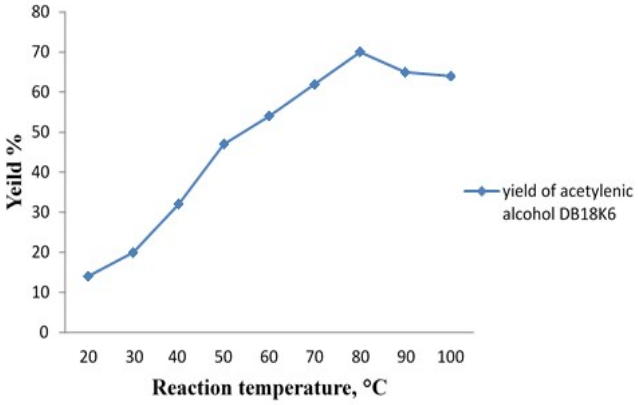


Figure 3. Dependence of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 on the reaction temperature.

The mathematical model faces the task of determining the relationship and the mathematical dependence of the product yield y as a function of f(x) - the reaction time. The analytical dependence y= f(x) is connected by the variables x and y.

To solve this problem, we use one of the methods of analytical dependence - the method of least squares.

The Table 1 shows the results of experimental data on the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6, where y_1 is the yield of the target product, t_1 is the reaction temperature (Fig. 3).

The analytical dependence of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 y, and the reaction temperature t, has the form:

$$y = at^3 + bt^2 + ct + d \ , \quad (7)$$

where *a, b, c, d* - coefficients leading to changes in the yield of the target acetylenic alcohol depending on temperature.

The sum of squared deviations for given parameters with coefficients - should be kept to a minimum:

$$E(a,b,c,d) = \sum_{i=1}^{9} [y_i - at_i^3 - bt_i^2 - ct_i - d]^2 = min \quad (8)$$

With respect to the given parameters, the partial derivatives of the function E(a, b, c, d) have the form:

$$\frac{\partial E(a,b,c,d)}{\partial a} = 2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i^3) \quad (9)$$

$$\frac{\partial E(a,b,c,d)}{\partial b} = 2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i^2) \quad (10)$$

$$\frac{\partial E(a,b,c,d)}{\partial c} = 2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i) \quad (11)$$

$$\frac{\partial E(a,b,c,d)}{\partial d} = 2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-1) \quad (12)$$

Let us represent the extremum of the function of parameters a, b, c and d equal to zero:

$$\frac{\partial E(a,b,c,d)}{\partial a} = 0 \ , \quad (13)$$

$$\frac{\partial E(a,b,c,d)}{\partial b} = 0 \ , \quad (14)$$

$$\frac{\partial E(a,b,c,d)}{\partial c} = 0 \ , \quad (15)$$

.

$$\frac{\partial E(a,b,c,d)}{\partial d} = 0 \quad (16)$$

Transforming the equations we get:

$$2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i^3) = 0 \quad (17)$$

$$2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i^2) = 0 \quad (18)$$

$$2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-t_i) = 0 \quad (19)$$

$$2\sum_{i=1}^{9}[y_i - at_i^3 - bt_i^2 - ct_i - d] \times (-1) = 0 \quad (20)$$

We bring this system of equations into the following form:

$$\sum_{i=1}^{9} t_i^6 a + \sum_{i=1}^{9} t_i^5 b + \sum_{i=1}^{9} t_i^4 c + \sum_{i=1}^{9} t_i^3 d = \sum_{i=1}^{n} y_i t_i^3 \quad (21)$$

$$\sum_{i=1}^{9} t_i^5 a + \sum_{i=1}^{9} t_i^4 b + \sum_{i=1}^{9} t_i^3 c + \sum_{i=1}^{9} t_i^2 d = \sum_{i=1}^{n} y_i t_i^2 \quad (22)$$

$$\sum_{i=1}^{9} t_i^4 a + \sum_{i=1}^{9} t_i^3 b + \sum_{i=1}^{9} t_i^2 c + \sum_{i=1}^{9} t_i d = \sum_{i=1}^{n} y_i t_i \quad (23)$$

$$\sum_{i=1}^{9} t_i^3 a + \sum_{i=1}^{9} t_i^2 b + \sum_{i=1}^{9} t_i c + nd = \sum_{i=1}^{n} y_i \quad (24)$$

To find the coefficients, we solve the matrix:

$$\begin{bmatrix} \sum_{i=1}^{9}(t_i)^6 & \sum_{i=1}^{9}(t_i)^5 & \sum_{i=1}^{9}(t_i)^4 & \sum_{i=1}^{9}(t_i)^3 \\ \sum_{i=1}^{9}(t_i)^5 & \sum_{i=1}^{9}(t_i)^4 & \sum_{i=1}^{9}(t_i)^3 & \sum_{i=1}^{9}(t_i)^2 \\ \sum_{i=1}^{9}(t_i)^4 & \sum_{i=1}^{9}(t_i)^3 & \sum_{i=1}^{9}(t_i)^2 & \sum_{i=1}^{9} t_i \\ \sum_{i=1}^{9}(t_i)^3 & \sum_{i=1}^{9}(t_i)^2 & \sum_{i=1}^{9} t_i & 9 \end{bmatrix} \begin{bmatrix} \sum_{i=1}^{9} y_i \cdot (t_i)^3 \\ \sum_{i=1}^{9} y_i \cdot (t_i)^2 \\ \sum_{i=1}^{9} y_i \cdot t_i \\ \sum_{i=1}^{9} y_i \end{bmatrix} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \quad (25)$$

The value n indicates the number of experiments performed at different temperatures, for a given synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 temperature range 20-100 °C, n=9 .

Let's simplify the temperature value by introducing the variable t', which will reduce the temperature value by a factor of 10 to:

$$t' = \frac{t}{10} \quad . \quad (26)$$

Then, the definition of the given coefficients a, b, c and d has the form of the following analytical dependence:

$$y = at'^3 + bt'^2 + ct' + d \quad (27)$$

Let us compose a system of linear algebraic equations for given coefficients:

$$\begin{cases} 2293433a+262038{,}1b+32069{,}20c+4055{,}764d = 112941{,}7 \\ 262038{,}1a+32069{,}20b+4055.764c+538{,}14d = 16672.04 \\ 32069{,}20a+4055{,}764b+538{,}14c+76{,}4d = 2550{,}2 \\ 4055{,}764a+538{,}14b+76{,}4c+12d = 410 \end{cases} \quad (28)$$

Solving the system of these equations for a, b, c and d, we obtain the values of the required parameters.

$$a = -0{,}104;\ b = 1{,}858;\ c = -5{,}60;\ d = 11{,}464 \quad (29)$$

Thus, the analytical temperature dependence of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 has the form:

$$y = -0{,}104t'^3 + 1{,}858t'^2 - 5{,}60t' + 11{,}464. \quad (30)$$

To compare the experimental data with the obtained parameters of the analytical dependence, we present the results of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 in Table 2.

Table 2

Comparative data (calculated and experimental) dependence of the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 on temperature

№	Temperature, *t*	Temperature, °C	Experimental data	calculated data
1	20	2	14	16.422
2	30	3	20	27.371
3	40	4	32	38.014
4	50	5	47	49.680
5	60	6	54	58.159
6	70	7	62	67.725
7	**80**	**8**	**70**	**72.456**
8	90	9	65	69.852
9	100	10	64	65.578

For visual comparison of the experimental and calculated data on the yields of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6, a graph was plotted (Fig. 4):

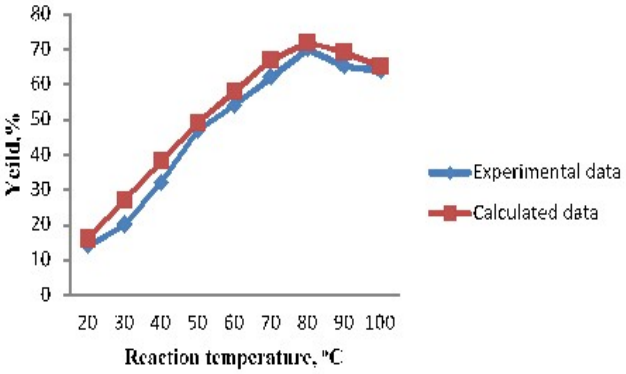


Figure 4. Comparison of experimental and calculated yield data for 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6.

When comparing the data in Table 2, the constructed analytical dependence

$$y = –0,104t'^3+1,858t'^2–5,60t'+11,464 \quad (31)$$

describes the chemical process for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 satisfactorily.

Previously, a time variable was introduced. Now, based on the obtained analytical dependence (3), the analytical formula for the variable t has the form

$$y = –0,1043+1,8582–5,60+11,464 \quad (32)$$

or

$$y = –0,000104t^3+0,01858t^2–0,560t+11,464 \quad (33)$$

Conclusion

A mathematical model for the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6 was created, the optimum synthesis, analytical dependences of the rate and yield of the reaction product depending on time were determined and reaction temperature.

A mathematical formula is proposed to describe the yield of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6. The experimental data correlates with the calculated ones. The proposed mathematical model makes it possible to predict the kinetics and conditions of the process. If necessary, this model can be supplemented with new required ratios to obtain more accurate quantitative characteristics of the synthesis of 4′,4′′-di-(1-methyl-1-hydroxy-2-phenylethynyl)-dibenzo-18-crown-6.

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