

# Physicochemical modeling of reactive violet 5 dye adsorption on home-made cocoa shell and commercial activated carbons using the statistical physics theory



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## ABSTRACT

Two equilibrium models based on statistical physics, i.e., *monolayer model with single energy* and *multilayer model with saturation*, were developed and employed to access the steric and energetic aspects in the adsorption of reactive violet 5 dye (RV-5) on cocoa shell activated carbon (AC) and commercial activated carbon (CAC), at different temperatures (from 298 to 323 K). The results showed that the *multilayer model with saturation* was able to represent the adsorption system. This model assumes that the adsorption occurs by a formation of certain number of layers. The  $n$  values ranged from 1.10 to 2.98, indicating that the adsorbate molecules interacted in an inclined position on the adsorbent surface and aggregate in solution. The study of the total number of the formed layers ( $1 + L_2$ ) showed that the steric hindrance is the dominant factor. The description of the adsorbate–adsorbent interactions by calculation of the adsorption energy indicated that the process occurred by physisorption in nature, since the values were lower than  $40 \text{ kJ mol}^{-1}$ .

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## Introduction

With the population growth, there is an increase in the demand for industrial products. A number of industries such as textile, food, food stuffs, cosmetic, pharmaceuticals products, rubber and leather, etc., apply dyes in their final products [1,2]. The production and consumption of these industrial products result in large amounts of wastewater contaminated with dyes [3,4]. Industrial wastewater contaminated with dyes is unsafe for aquatic life, impeding light penetration and reducing the photosynthetic activity of aquatic plants [5]. The presence of dyes in the environment affects all living organisms because they have toxic and carcinogenic properties [6–8]. Therefore, it is necessary the removal of synthetic dyes from aqueous effluents.

Adsorption is one of the most employed operations for removal of dyes from industrial effluents [6–9]. Although the adsorption operation is largely used, the adsorption equilibrium still requires further elucidation. To understand the adsorption process at a first

time, classical interpretations were developed using empirical models describing the adsorption process of the two considered systems (RV-5 and activated carbons) [10]. To interpret microscopically the adsorption of reactive violet 5 dye (RV-5) on cocoa shell activated carbon (AC) and commercial activated carbon (CAC) at different temperatures, a simple model named *monolayer model with single energy* [11] and a *multilayer model with saturation* [11,12], derived from statistical physics elements, were chosen and developed in this paper. The first model represents the general case of Langmuir model, assuming that a site contains  $n$  molecules and a formation of only one layer occurs. The second model, assumes that the adsorption occurs by a formation of  $1 + L_2$  layers. It is possible to select other statistical physics models to test the adsorption isotherms, for example, double or triple layer models, but, all these models are tested indirectly, since are included in the *multilayer model with saturation*. In this paper and based on the simulations results, all the adsorption isotherms were interpreted using the *multilayer layer model with saturation*.

This work aimed to study the physicochemical modeling of reactive violet 5 dye adsorption on home-made and commercial activated carbons, using the adequate model in order to describe

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the dyes behavior in solution by estimation of the aggregation degree of the dye molecules based on theoretical observations, and to deduce approximately the total number of the formed layers on the adsorbent surface.

## Materials and methods

### Solutions and reagents

The RV-5 dye (CAS 12226-38-9; C.I. 18097;  $C_{20}H_{16}N_3O_{15}S_4Na_3$ ,  $735.58 \text{ g mol}^{-1}$ ,  $\lambda_{\text{max}} = 545 \text{ nm}$  see [Supplementary Fig. 1](#)) with purity of 86%, was achieved from Sigma-Aldrich (São Paulo, Brazil) and was used without purification. A stock solution ( $5.0 \text{ g L}^{-1}$ ) of RV-5 dye was prepared by weighing a calculated amount of the dye and dissolving in deionised water. The stock solution was diluted to obtain various working solutions. The pH of the solutions was adjusted using a Digimed DM-22 pH meter, with a  $0.10 \text{ mol L}^{-1}$  NaOH and/or a  $0.10 \text{ mol L}^{-1}$  HCl.

### Adsorbents

Cocoa shell activated carbon (AC) and commercial activated carbon (CAC) were used in this work. Commercial activated carbon (CAC) was supplied by Vetec (325–400 mesh). The cocoa shell activated carbon adsorbent was prepared using the following procedures [10]: an amount of 70.0 g of biomass plus 70.0 g of inorganic components (20% lime, 40%  $ZnCl_2$ , and 40%  $FeCl_3$ ) and 45.0 mL of water were mixed to obtain a paste. This material was placed in a mould cylinder ( $253.34 \text{ cm}^3$ ), wet-shaped and dried at  $25 \text{ }^\circ\text{C}$  for 24 h. The dried cylinder was inserted in a stainless steel reactor [10]. The reactor was thereafter heated in the tubular furnace at  $10 \text{ }^\circ\text{C min}^{-1}$  up to  $750 \text{ }^\circ\text{C}$  for 30 min, under  $N_2$  atmosphere ( $100 \text{ mL min}^{-1}$ ). The adsorbent was later cooled down to room temperature under  $N_2$  ( $25 \text{ mL min}^{-1}$ ), milled, sieved to a particle size  $\leq 103 \text{ }\mu\text{m}$  and stored until use. This carbon material was named CC. To complete the chemical activation of the carbon, a leaching procedure described in the literature was employed [10], obtaining the cocoa shell activated carbon AC.

### Batch adsorption studies

The adsorption capacity of proposed AC was compared with a well-established CAC. 50.0 mg of adsorbent and a 20.0 mL of RV-5 dye solution ( $300.0\text{--}1500.0 \text{ mg L}^{-1}$ ) were placed in various 50.0 mL Falcon tubes at different pH values (2.0–10.0). The mixtures were agitated between 5 and 480 min inside a thermostatic shaker (Oxylab, São Leopoldo, Brazil) from 298 to 323 K. The mixtures were centrifuged for 5 min at 10,000 rpm after the batch adsorption experiments, to separate the adsorbents from the dye solutions. When necessary, aliquots of the supernatant were diluted with deionised water at pH 2.0 before spectroscopic measurement. UV/visible spectrophotometer T90+ UV-VIS was used to quantify the final RV-5 concentration in solution, after adsorption at a maximum wavelength of 545 nm.

## Adsorption models development and simulation

Generally, the adsorption isotherms form plays an important role to retrieve helpful information's in order to choose the adequate models suitable for simulation. All the adsorption isotherms of RV-5 dye on activated carbon (AC) and on a commercial activated (CAC) carbon are characterized by a simple form showing that a saturation phenomenon was appeared at high concentration, reflecting that the adsorption is finished. So, the adsorption process of RV-5 dye occurred by a formation of one layer or by a certain

number of layers on the adsorbent surfaces. For the reason, two statistical physics models were selected to simulate the adsorption isotherms at different temperatures. The first selected model named by 'monolayer model with single energy' (**model 1**) [11], it is a simple model describing the adsorption by a formation of one layer on the adsorbent surface. It is possible also to select other models describing the adsorption of RV-5 dye by a formation of two and three layers for example, but other important statistical physics model was selected gathering all these cases named by 'multilayer model with saturation' (**model 2**) [12]. The second selected model describes the adsorption process with a formation of certain number of layers.

To develop the two adsorption models, certain hypotheses were applied: the interaction between the dye molecules was neglected, because the concentrations are lower than the dye solubility [11–13]. In addition to this, the mutual interaction between the adsorbate dyes and solvent ones was also neglected [11–13]. These hypotheses were applied to facilitate the interpretations.

### Monolayer model with single energy

Firstly, it was supposed that the dye interact with the adsorption surface of AC and CAC by only one energy, and it was denoted as  $-\varepsilon$  [11,14]. We assumed also that the adsorption surface containing a certain number of identical receptor sites characterized by the  $N_M$  density [1,3]. Mathematically, the first step to calculate the model is to write the expression of the partition function of a single receptor site. According to other pervious works, this partition function of one receptor site is given by [11,13,15]:

$$z_{gc_1} = \sum_{N_i=0,1} e^{-\beta(-\varepsilon_i - \mu_i)N_i} = 1 + e^{\beta(\varepsilon + \mu)} \quad (1)$$

where,  $-\varepsilon_i$  ( $\text{kJ mol}^{-1}$ ) is the adsorption energy of the receptor site,  $\mu_i$  is the chemical potential of the adsorbed state ( $\text{kJ mol}^{-1}$ ),  $N_i$  is the receptor site occupation state,  $\beta$  is the Boltzmann factor and  $T$  the absolute temperature (K). This function contains two simple terms describing microscopically the dye behavior on the adsorption surface. If the partition function is equal to 1, we can deduce that the receptor site occupation state  $N_i$  is equal 0 indicating that the receptor site is empty. It is clear that the second term ( $e^{\beta(\varepsilon + \mu)}$ ) of the partition function showing that the receptor site is occupied. It is easy now to write the partition function in relation with the total receptor site ( $N_M$  density ( $\text{mg g}^{-1}$ )) [11,12].

$$z_{gc_1} = (z_{gc})^{N_M} \quad (2)$$

According to other previous works, the expression of the occupied sites is given by [11,13]:

$$N_{01} = \frac{N_M}{1 + \left(\frac{c_{1/2}}{c}\right)^n} \quad (3)$$

The expression of the first selected model for simulation is given by [11]:

$$Q_1 = \frac{nN_M}{1 + \left(\frac{c_{1/2}}{c}\right)^n} \quad (4)$$

being,  $Q_1$  the adsorbed mass ( $\text{mg g}^{-1}$ ),  $n$  the number of molecules per site,  $c_{1/2}$  the concentration at half saturation ( $\text{mg L}^{-1}$ ) and  $c$  ( $\text{mg L}^{-1}$ ) the equilibrium concentration.

### Multilayer model with saturation

The second model describes the dyes adsorption with a formation of a limited number of layers.

To calculate the expression of this model, we assume that the RV-5 dye of the first layer interact with the adsorbent surface of

AC and CAC by the energy  $(-\varepsilon_1)$  [11,12]. In addition to the first layer, we supposed that the RV-5 dye were assumed to be interact on  $L_2$  other layers with  $(-\varepsilon_2)$  energy [11,12]. Microscopically, the partition function of one receptor site according to the these hypotheses is given by [11,12]:

$$Z_{gc_2} = 1 + e^{\beta(\varepsilon_1+\mu)} + e^{\beta(\varepsilon_1+\varepsilon_2+2\mu)} \frac{1 - (e^{\beta(\varepsilon_2+\mu)})^{L_2}}{1 - e^{\beta(\varepsilon_2+\mu)}} \quad (5)$$

As the first expression, this function contains also two terms: the first term  $(1 + e^{\beta(\varepsilon_1+\mu)})$  is similar to the first partition function ( $Z_{gc1}$ ) of the model 1 describing the adsorption of RV-5 dye by a formation of the first layer. The second term  $(e^{\beta(\varepsilon_1+\varepsilon_2+2\mu)} \frac{1 - (e^{\beta(\varepsilon_2+\mu)})^{L_2}}{1 - e^{\beta(\varepsilon_2+\mu)}})$  describes the adsorption by a formation of certain number of layers characterized by the  $L_2$  layer. So the total number of layers is  $1 + L_2$ .

The expression of the second model is given by [11,12]:

$$Q = nN_M[F_1(c) + F_2(c) + F_3(c) + F_4(c)]/[G(c)] \quad (6)$$

where,  $F_1(c)$ ,  $F_2(c)$ ,  $F_3(c)$ ,  $F_4(c)$  and  $G(c)$  are given by:

$$F_1(c) = -\frac{2(\frac{c}{c_1})^{2n}}{(1 - (\frac{c}{c_1})^n)^2} + \frac{(\frac{c}{c_1})^n(1 - (\frac{c}{c_1})^{2n})}{(1 - (\frac{c}{c_1})^n)^2} \quad (7)$$

$$F_2(c) = \frac{2(\frac{c}{c_1})^n(\frac{c}{c_2})^n(1 - (\frac{c}{c_2})^{nN_2})}{(1 - (\frac{c}{c_2})^n)^2} \quad (8)$$

$$F_3(c) = -\frac{(\frac{c}{c_1})^n(\frac{c}{c_2})^n(\frac{c}{c_2})^{nN_2}N_2}{(1 - (\frac{c}{c_2})^n)^2} \quad (9)$$

$$F_4(c) = \frac{(\frac{c}{c_1})^n(\frac{c}{c_2})^{2n}(1 - (\frac{c}{c_2})^{nN_2})}{(1 - (\frac{c}{c_2})^n)^2} \quad (10)$$

$$G(c) = \frac{(1 - (\frac{c}{c_1})^{2n})}{(1 - (\frac{c}{c_1})^n)^2} + \frac{(\frac{c}{c_1})^n(\frac{c}{c_2})^n(1 - (\frac{c}{c_2})^{nN_2})}{(1 - (\frac{c}{c_2})^n)^2} \quad (11)$$

The application of a simple simulation program based on Levenberg–Marquardt algorithm (LMA) leads to fit the adsorption isotherms and to retrieve the  $R^2$  (coefficient of determination) and  $RMSE$  (estimated standard error) values which represent two criterions to select the adequate model. All the simulation results showed that no strongly difference between the  $R^2$  (0.996–0.999) and  $RMSE$  (3.11–7.24) values of the two models, but the parameter values of the multilayer model saturation vary with a clear manner with temperature, contrary to the parameters values of the first model which vary as function of temperature with a not clear

manner which can pose a problem in interpretation. Consequently, the multilayer model with saturation model was selected to interpret the adsorption systems. All the simulation of the adsorption isotherms of RV-5 on AC and CAC are reported in Fig. 1.

### Model parameters interpretation

In this section, we try to interpret the adsorption isotherms by the model parameters. The usefulness of the parameters meaning plays in general an important role to understand the adsorption process. In terms of interpretation, the  $n$  parameter plays two important roles: Geometrically, this parameter describes the adsorption position of RV-5 dye on the adsorbent surface as function of their values deduced by numerical simulation. Indeed, if this value is inferior to 1, we can attribute a simple definition of this parameter describing the portion of the adsorbed molecule per site explaining a horizontal docking [11,12,16] on the adsorbent surface and showing that the adsorption is multi-docking process [11,12,16]. The second case, if the  $n$  parameter value is superior to 1: it represents the number of docked molecules which interact with one receptor site describing a multi-molecular process. In this case, we can understand that the dye molecules interact with an inclined position with the adsorbent surface. The second aspect describes the aggregation phenomena and their degree of the adsorbate molecules in solution [11,12,16]. The evolution of this parameter is reported in Fig. 2.

Referring to the values of this parameter (Fig. 2), we noticed that the values are always superior to the unity at different temperatures, which explain the aggregation of RV-5 dye in solution. Based on this information, the adsorption of RV-5 dye is multi-molecular regardless of the adsorbent nature and the dye molecules interact in an inclined position. The  $n$  values of dye for the two studied systems vary between 1.10 and 2.98 indicating that the aggregation degree varies between 1 and 3 (monomer;  $n \sim 1$ , dimer;  $n \sim 2$  and trimer;  $n \sim 3$ ). Chemically, we can exploit the dye aggregation by the simple reaction:  $D \rightarrow D_n$  [17] which indicates that is an endothermic reaction before the adsorption (in solution).

In terms of comparison, the  $n$  values of the two studied systems, we noticed that the number of molecules per site of RV-5 dye on AC is higher than the number of molecules per site of RV-5 dye on CAC at different temperatures. The results can be explained by the higher affinity of the functional group's which contribute in the adsorption of RV-5 on AC. In general the interpretation of the number of molecules per site leads to interpret easily the density of the receptor sites. The  $N_M$  evolution is reported in Fig. 3. This figure shows a clear decrease with temperature. This decrease is mainly due to the increase of the number of molecules per site as function of temperature. In other words, the aggregation

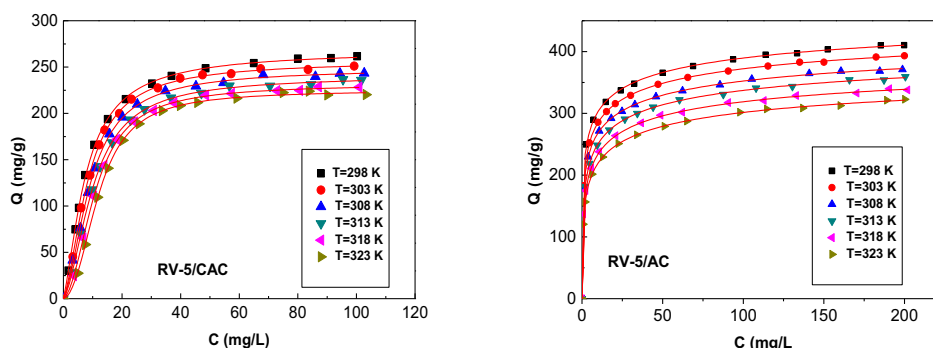


Fig. 1. Fitting of adsorption isotherms of RV-5 on AC and CAC at different temperatures.

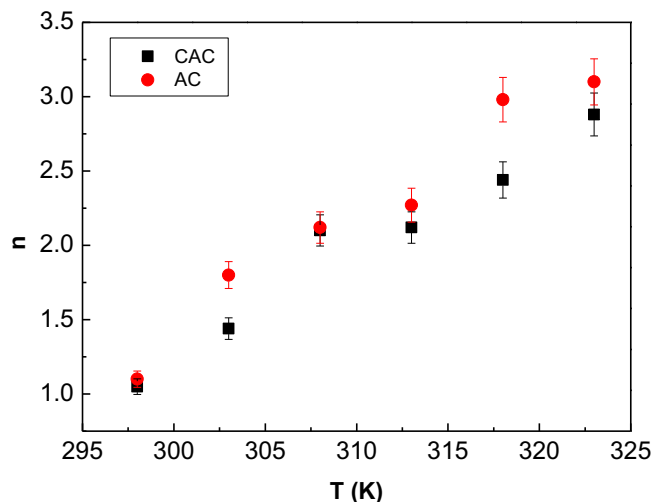


Fig. 2. Evolution of  $n$  parameter with temperature.

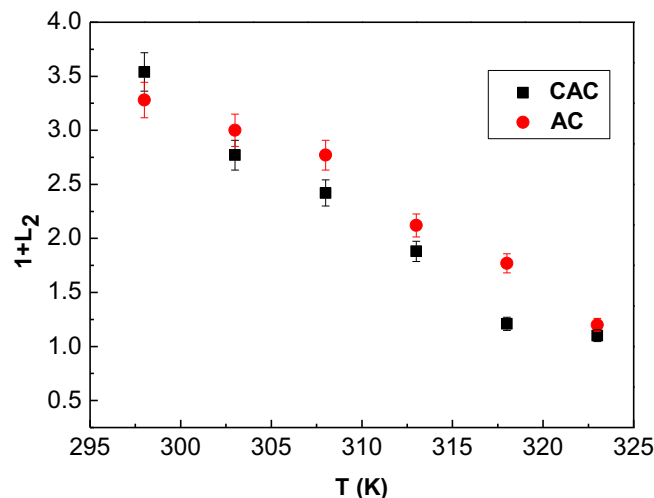


Fig. 4. Evolution of  $1 + L_2$  layers with temperature.

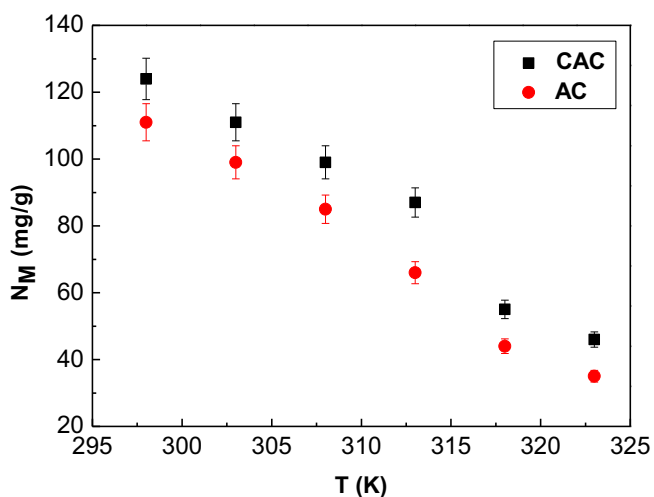


Fig. 3. Evolution of  $N_M$  parameter with temperature.

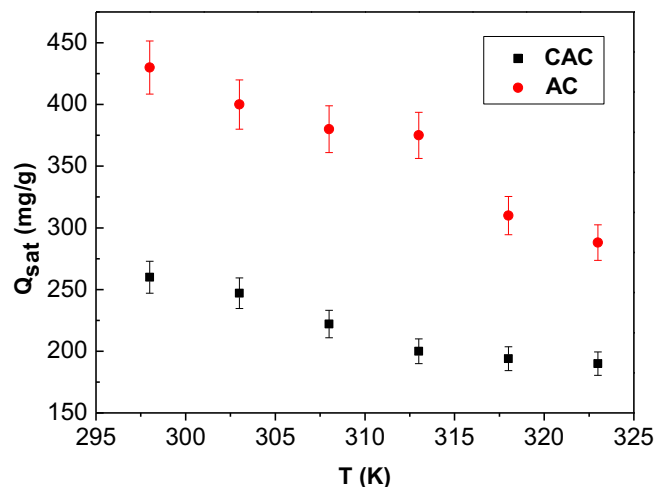


Fig. 5. Adsorbed quantity evolution as function of temperature.

phenomenon controlled the  $N_M$  evolution. Indeed, the increase of  $n$  parameter makes a limited space on the adsorbent surface to accept other molecules which explains the decrease of the  $N_M$  parameter.

The number of the total formed layers evolution is presented in Fig. 4. As a first consequence, we noticed that the number of the total formed layers ( $1 + L_2$ ) is relatively low for the two studied systems which are probably due to the steric hindrance effect [11]. This steric hindrance effect stops the formation of the layers. By a simple analysis of this adjustable parameter values, we noticed that the adsorption process occurred by a formation of 3.54 and 3.28 layers for AC and CAC respectively. This model parameter is important which shows approximately the total number of the formed layers contrary to the other models developed in literature.

The last model parameter is the total adsorbed quantity at saturation which depends on the other model parameters described above ( $Q_{sat} = nN_M (1 + L_2)$ ). This parameter evolution is reported in Fig. 5. Based on this figure, we noticed that the AC is the best adsorbent since all their adsorbed quantity values are higher than CAC. The  $n$  and  $1 + L_2$  parameter values of the RV-5 adsorption on AC are superior to values of RV-5 adsorption on CAC. This difference of the two parameter values can explain the difference between the adsorbed quantities.

## Discussion and adsorption energy

Energetically, the process of RV-5 dyes was governed by two different energies describing the behavior of the dye molecules before and after the adsorption process: activation energy and adsorption energy. Referring to the evolution of the number of molecules per site (Fig. 2) of RV-5 dye as function of temperature and their magnitude, it is clear that the temperature has a major effect since this number increases always and is characterized by a linear trend. Simply, we can understand that the adsorption systems are thermally activated and the activation energy is the dominant factor which is responsible on the aggregation phenomenon. Regarding now the low aggregation degree ( $1 < n < 3$ ), which may explain by the low interactions between the dyes in solution. To characterize the interactions between the aggregate molecules and the adsorbent, it is necessary to estimate the adsorption energy values using the simple equation:  $-\Delta E = -RT \ln(c_s/c_{1/2})$  [11,16] ( $c_s$  is the dye solubility and  $c_{1/2}$  is the concentration at half saturation). Based on the adsorption energy evolution (Fig. 6), the first result indicates that these interactions are low, since all the adsorption energy values were inferior to  $40 \text{ kJ mol}^{-1}$  [17–19]. The lowest values of these energies are probably due to the lowest values of the formed layers. So, the adsorption process is

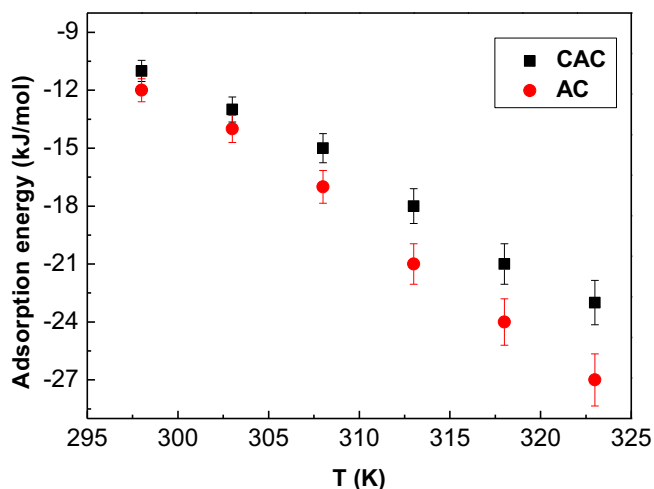


Fig. 6. Adsorption energy evolution with temperature.

physisorption. The negative values explaining that this process is exothermic, in agreement with the literature [17–19]. The decrease of the energy as function of temperature is due to the decreases of the adsorbed quantity.

## Conclusion

The multilayer model with saturation developed using a statistical physics approach was selected to attribute microscopic interpretations of RV-5 dye on two adsorbents. Based on the study of the model parameters, some conclusions were obtained. The  $n$  parameter ranged from 1.10 to 2.98, showing that the dye aggregate in solution and, the interactions occurred in an inclined position on the adsorbent surface. The steric hindrance effect explains the lowest values of the total numbers of the formed layers on AC and CAC. From the energetic viewpoint, all the adsorption energy values were lower than  $40 \text{ kJ mol}^{-1}$ , indicating physisorption. The negative values of adsorption energy showed that this process is exothermic.

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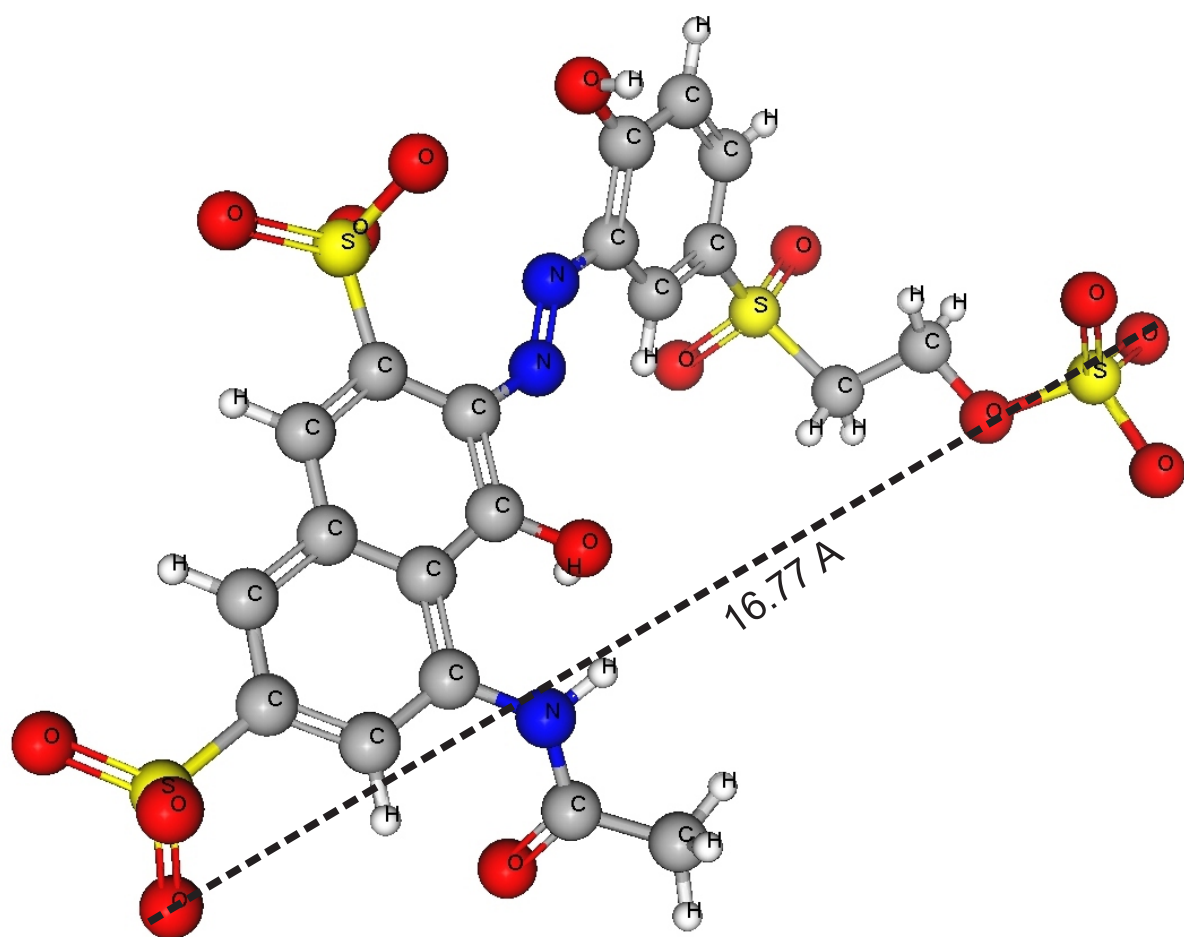
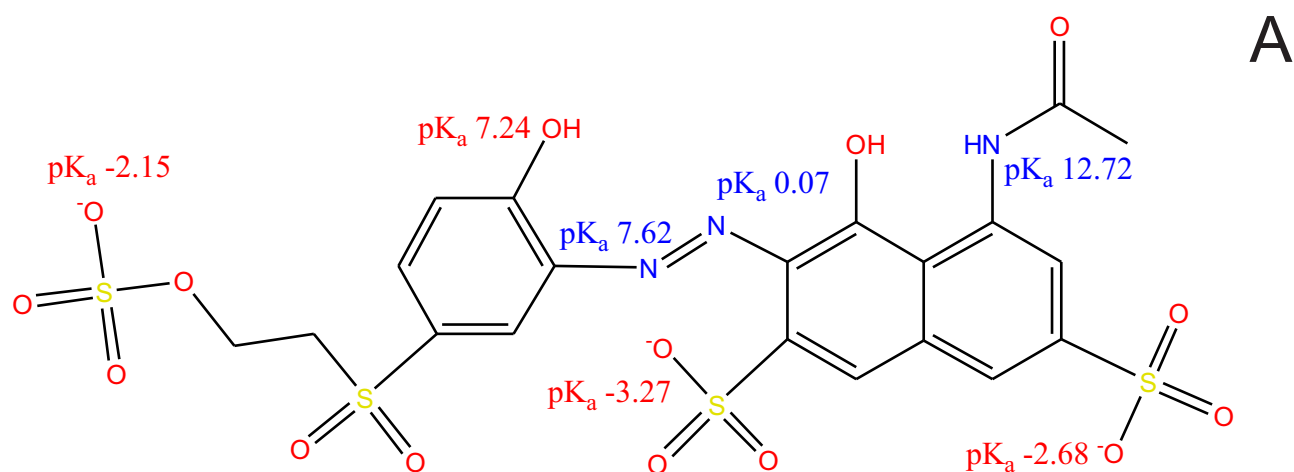
## Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.rinp.2016.12.014>.

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**Supplementary Fig 1: (A) Structural formula of RV-5; (B) Optimized three-dimensional structural formula of RV-5.** The dimensions of the chemical molecule were calculated using MarvinSketch version 16.9.5.0. Van der Waals surface area = 781.17 Å<sup>2</sup> (pH 6.7-10.1); Polar surface area 345.60 Å<sup>2</sup> (pH 6.7-10.1); Van der Waals volume 483.47 Å<sup>3</sup>; Dipole Moment 19.00 Debye, hydrophobic-lipophilic balance 82.67, Log P