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1,2,3,4-Tetrahydropyrimidine Derivative for Selective and Fast Uptake of Cadmium Ions from Aqueous Solution

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Abstract: The aim of this work was to evaluate the performance of a 1,2,3,4-tetrahydropyrimidine derivative as a powerful heterocyclic compound for the elimination of Cd(II) ions from aqueous solutions. The tetrahydropyrimidine derivative was prepared during 30 min of milling by planetary ball mill with a ball-to-powder mass ratio of 8:1 and a rotation speed of 750 rpm. Nuclear magnetic resonance (NMR) and infrared (IR) were used to identify the obtained tetrahydropyrimidine derivatives. Furthermore, batches of experiments were carried out to establish the adsorption equilibrium, kinetics, and thermodynamic variables of the tetrahydropyrimidine derivatives for toxic heavy Cd(II) ions. The adsorption data were simulated by applying the Langmuir manner, the Freundlich equation, the pseudo-first-order and pseudo-second-order equations. The adsorption procedure was discovered to be very influenced by PH. The removal of heavy metal ions reached a maximum value quickly within 6 min and the adsorption data better adjusted the Langmuir isotherm than that of the Freundlich isotherm. The maximum Cd(II) ions adsorption capacity was approximated to be 151.16 mg g^{-1} at 328 K and a pH of 6 to 7. It was found that the adsorption kinetics of Cd(II) ions obeyed pseudo-second-order adsorption kinetics. The examination of the thermodynamic variables of tetrahydropyrimidine derivative showed a spontaneous endothermic adsorption procedure. Otherwise, positive entropy values put forward a rise in the randomness at the solid-solution interface when heavy metal ions are adsorbed.

Keywords: 1,2,3,4-tetrahydropyrimidine derivative; ball milling; heavy metal; Cd(II) ion; adsorption; kinetics; thermodynamics

1. Introduction

Currently, the global pollution rate is increasing due to many different factors, such as the high heavy metal discharge concentrations from industries. In addition to other toxic heavy metals such as lead and copper, cadmium is a highly toxic heavy metal and is known as one of the most dangerous to human health. In addition, cadmium is not biodegradable, and exposure to this pollutant can lead to various diseases and disorders [1]. The method commonly used to solve these serious environmental problems is adsorption, which has been proven to be one of the most efficient and cost-effective methods for water treatment applications [2]. However, the real problem in this area is the choice of selecting new adsorbents.

Various adsorbents have been applied to remove the ions of heavy metal, such as activated carbon [3], clays [4,5], zeolites [6–8], and agricultural residues [9–12]. Moreover, the major drawbacks of these adsorbents are their low adsorption capacity and their difficulties in separating some of them

from water. Recently, special attention has been given to the organic-inorganic hybrid polymers and functionalized polymers as attractive absorbents, due to their high efficiency for the removal of heavy metals from contaminated water [13–27]. In these mixtures, the organic compounds are combined with inorganic substrates, which provide a high interaction with selected metal ions and relatively high adsorption capacities of the metal ions. Functionalized and hybrid polymeric materials often exhibit the best properties and exhibit high performance in terms of physical, chemical, and mechanical properties [28].

This research paper focuses on the efficiency and selectivity of the organic heterocyclic compound (1,2,3,4-tetrahydropyrimidine derivative) as a promising adsorbent for the uptake of Cd(II) ions from aqueous solutions. The pyrimidine derivative was prepared by planetary ball mill as a green synthesis technique, and its structure was confirmed by nuclear magnetic resonance (NMR) and infrared (IR). The effects of initial pH, temperature, and initial concentration on Cd(II) removal were studied. Mathematical models were also investigated, including the Langmuir and Freundlich models for the sorption isotherm data, and the kinetics data (first and second order equations). The rate constants, the adsorption capacities, and the thermodynamic variations (ΔH^0, ΔS^0 and ΔG^0) were also assessed and discussed.

2. Materials and Methods

All the organic reagents (benzaldehyde, ethyl acetoacetate, urea) used in this work were purchased from Sigma-Aldrich (St Louis, MO, USA). The ball milling apparatus used in this study was a Planetary Micro Mill PULVERISETTE 7 (Fritsch, Idar-Oberstein, Germany) classic line equipped with tempered steel bowls of 45 mL and tempered steel grinding balls of 10 mm. The melting point was determined with a Stuart SMP10 melting point equipment (Bibby Scientific Staffordshire, UK). IR spectra were provided by an FT-IR-Tensor 27 spectrometer (Bruker, Ettlingen, Germany) in KBr pellets. ^{1}H and ^{13}C-NMR spectra were obtained using a Bruker 400 NMR spectrometer (Bruker Biopsin, Rheinstetten, Germany) in DMSO-d6 with TMS as the internal standard. Chemical shifts were indicated in units of parts per million (ppm).

2.1. Synthesis of Ethyl 6-Methyl-2-oxo-4-Phenyl-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate (4)

The 1,2,3,4-tetrahydropyrimidine compound (4) (Figure 1) was synthesized according to the reference [29]. Equimolar amounts of benzaldehyde (1), ethyl acetoacetate (2), and urea (3) were placed into tempered steel vials with tempered steel balls (10 mm in diameter) in a Planetary Micro Mill Pulverisette 7. The ball-to-reagent weight ratio equals 8:1, and the Planetary Micro Mill was set to 750 rpm. The 1,2,3,4-dihydropyrimidine product (4) was obtained in pure form after 30 min of milling without further purification. The structure of the synthesized product (4) was confirmed by NMR (^{1}H and ^{13}C)) and IR analysis (Figures 2 and 3).
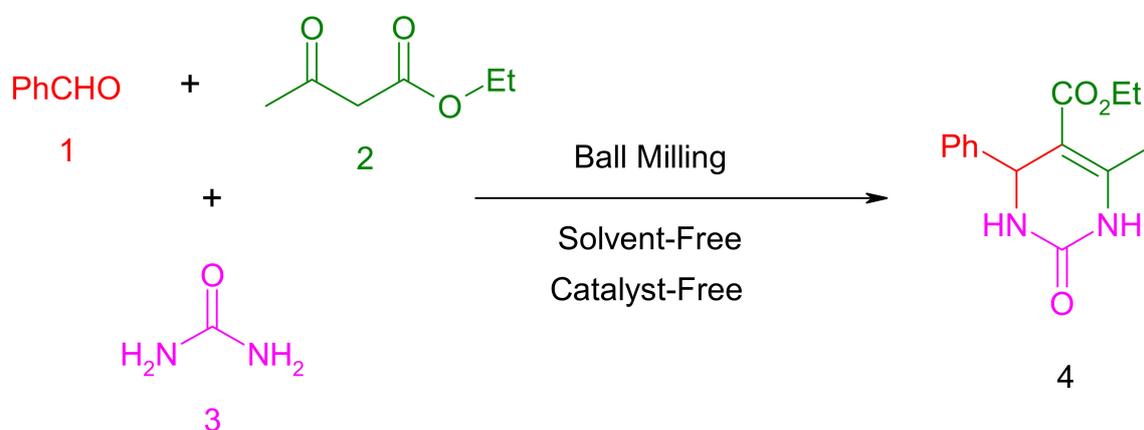

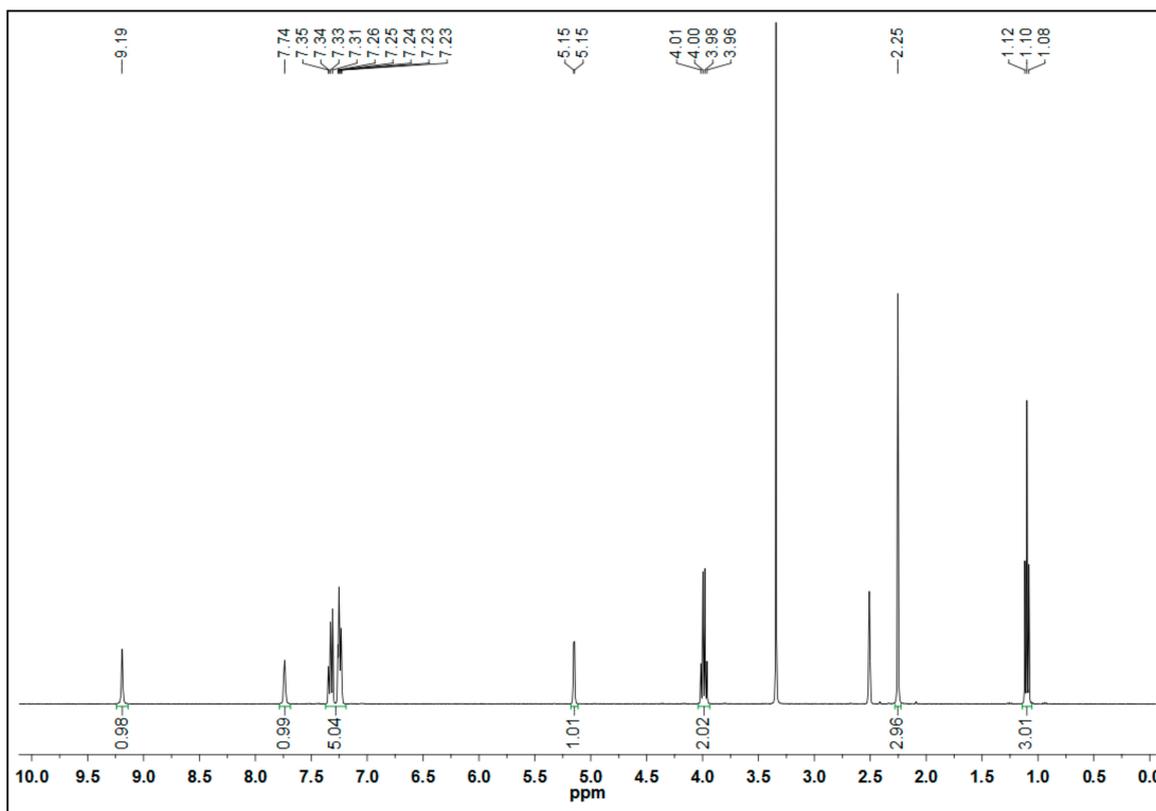**Figure 1.** The 1,2,3,4-tetrahydropyrimidine derivative synthesis under ball milling.

Figure 2. ^{1}H-nuclear magnetic resonance (NMR) spectrum of 1,2,3,4-tetrahydropyrimidine derivative 4.
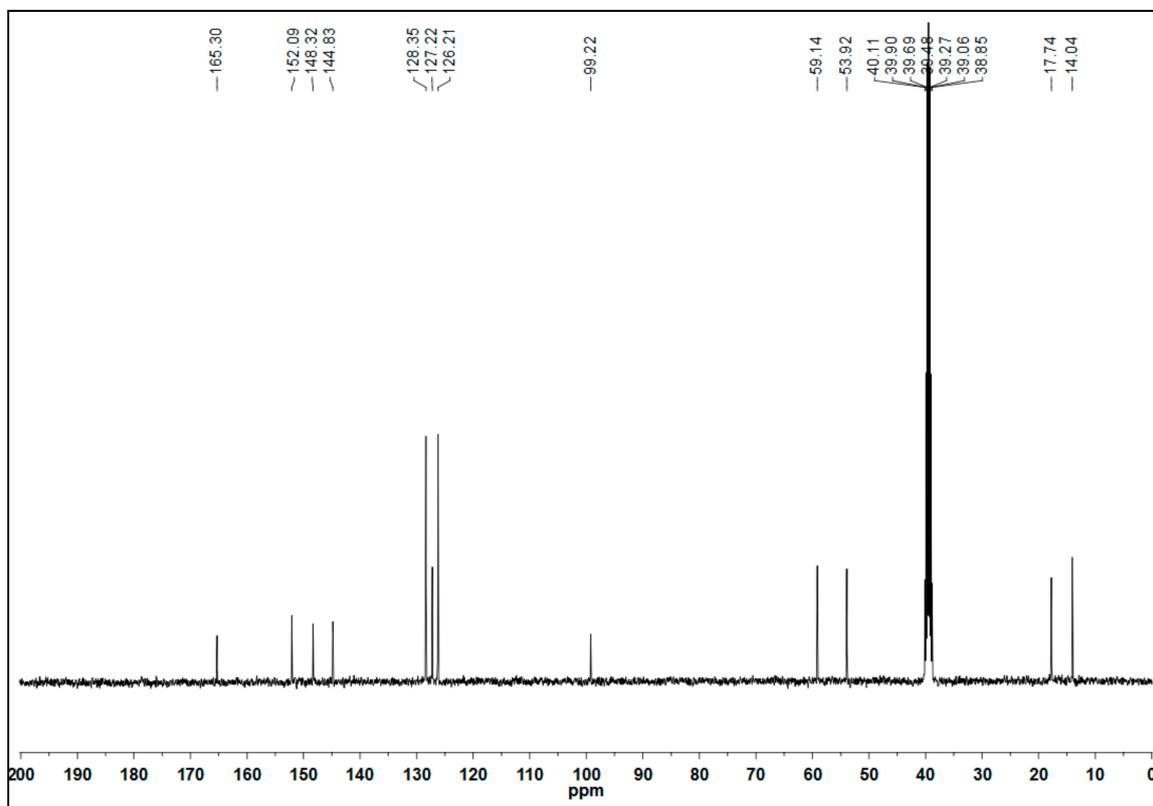

Figure 3. ^{13}C-nuclear magnetic resonance (NMR) spectrum of 1,2,3,4-tetrahydropyrimidine derivative 4.

2.2. Characteristic Data of Ethyl 6-Methyl-2-oxo-4-Phenyl-1,2,3,4-Tetrahydropyrimidine-5-Carboxylate (4)

IR (KBr, νmax, cm^{-1}): 3228, 3240.2, 3116.8, 29781.7, 1701.1, 1647.1. ^{1}H-NMR (400 MHz, DMSO-d6) δ 9.19 (s, 1H), 7.74 (s, 1H), 7.37–7.19 (m, 5H), 5.15 (d, J = 3.3 Hz, 1H), 3.99 (q, J = 7.1 Hz, 2H), 2.28 (s, 1H), 1.10 (t, J = 7.1 Hz, 3H); ^{13}C-NMR (100 MHz, DMSO-d6) δ 165.30, 152.09, 148.32, 144.83, 128.35, 127.22, 126.21, 99.22, 59.14, 53.92, 17.74, 14.04.

2.3. Adsorption Procedure

2.3.1. Preparation of Cd(II) Ion Solutions

The (1000 mg L^{-1}) stock solution of Cd(II) was made by dissolving necessary amounts of cadmium nitrate (Cd(NO$_3$)$_2$), in distilled water. Experimental solutions at the required concentration were then achieved by successive dilutions. All the reagents were of analytical category, purchased from Sigma-Aldrich (St Louis, MO, USA) and were used as received without further purification [30].

2.3.2. Analysis of Cd(II) Ion Adsorption

In order to investigate the adsorption performance of the adsorbent towards Cd(II), many experiments were performed in batch mode by mixing together 10 mg of 1,2,3,4-tetrahydropyrimidine compound (4) and 25 mL of ionic cadmium solution in a 50 mL glass vial with a known pH and temperature. The initial concentration of cadmium ions was between 20–160 mg L^{-1}, the pH values from 3.0 to 10.0, and the temperature from 298 to 318 K. The mixed amounts were stirred continuously with a shaker at 600 rpm for 12 h. A 15 mL of the suspension was withdrawn from each flask, centrifuged at 6000 rpm for 10 min, and also filtered through 0.45 μm cellulose acetate syringe filter. The concentrations of Cd(II) were analyzed with an atomic emission spectrometry (Spectro genesus ICP-OES). All the experimentation were carried out twice, and the average values are used in this work.

According to Equation (1), the mass (mg) of Cd(II) removed by 1 g of the adsorbent, q_e, is:

$$q_e = \frac{(C_0 - C_e) \cdot V}{m}, \tag{1}$$

where parameter C_0 represents the liquid phase initial concentration (mg L^{-1}), C_e is the cadmium ion aqueous-phase concentration after adsorption (mg L^{-1}), and V represents the volume of the pollutant solution (L), m is the mass of the dihydropyrimidine derivative.

The sorption data of cadmium ions are correlated to the theoretical models of Langmuir and Freundlich:

Langmuir equation

$$\frac{C_e}{q_e} = \frac{1}{Q_0} C_e + \frac{1}{Q_0 \cdot b}, \tag{2}$$

Freundlich equation

$$Ln(q_e) = \frac{1}{n} Ln(C_e) + Ln(k), \tag{3}$$

where C_e represents the equilibrium concentration of the solute in the solution (mg L^{-1}), q_e is the amount of cadmium ions adsorbed per unit weight of adsorbent (mg g^{-1}), Q_0 depicts the theoretical monolayer saturation capacity [31], and b accounts for the Langmuir equilibrium constant. The values of Q_0 and b can be graphically specified from the linearized and rearranged Langmuir expression (Equation (2)). k and n are constants allied to the strength of the adsorption and distribution bonds, respectively [32]. The values of k can be obtained graphically according to Langmuir equation (Equation (3)). The constant k can be defined as an adsorption coefficient which represented the quantity of adsorbed metal ion for a unit equilibrium concentration (i.e., C_e = 1). The slope, $1/n$, is a measure of the sorption intensity or surface heterogeneity [33]. the situation $1/n < 1$ is the most common

and corresponds to a normal L-type Langmuir isotherm, while $1/n > 1$ is indicative of a cooperative adsorption which involves strong interaction between the molecules of adsorbate [34], which involves strong interactions between the molecules of the adsorbate themselves. The essential characteristics of a Langmuir isotherm can be expressed in terms of a dimensionless separation factor, R_L, which describes the type of isotherm:

$$R_L = \frac{1}{1 + b \cdot C_0}, \tag{4}$$

where C_0 is the initial adsorbate concentration in the solution. The R_L indicates the shape of the isotherms to be either unfavorable ($R_L > 1$), favorable ($0 < R_L < 1$), linear ($R_L = 1$), or irreversible ($R_L = 0$). To envisage the adsorption data of Cd(II) as a function of time, two kinetic examples were suggested and tested: a pseudo-first-order and a pseudo-second order. The first-order method can be expressed linearly as follows:

$$\text{Ln}(q_e - q_t) = \text{Ln}(q_e) - k_1 \cdot t, \tag{5}$$

where q_e and q_t (in mg g^{-1}) represent the amount of Cd(II) adsorbed at equilibrium and at time t (min), respectively, and k_1 (min^{-1}) is the rate constant of first-order adsorption. The values of k_1 and q_e are deduced from the slope of the plot of $\text{Ln}(q_e - q_t)$ versus t, respectively.

The linear form of pseudo-second-order model is expressed as:

$$\frac{t}{q_t} = \frac{1}{k_2 \cdot q_e^2} + \frac{t}{q_e}, \tag{6}$$

where k_2 (g/mg min) represents the equilibrium rate constant of pseudo second-order adsorption. The plot t/qt versus t should be linear, when the pseudo-second-order models is adequate. The values of k_2 and q_e can be determined from the slope and intercept of the plot, t$_{1/2}$. The half adsorption time is the time intended to absorb half of the maximal amount of Cd(II) adsorbed at equilibrium. In the case of a pseudo-second-order process, the value of t$_{1/2}$ is calculated by the following relationship:

$$t_{1/2} = \frac{1}{k_2 \cdot q_e}. \tag{7}$$

The thermodynamic functions (ΔH^0, ΔS^0, and ΔG^0) for the adsorption of cadmium ions by dihydropyrimidine derivative were calculated using the subsequent equations:

$$\Delta G^0 = -RT\text{Ln}k_a, \tag{8}$$

$$\Delta S = \frac{\Delta H^0 - \Delta G^0}{T}, \tag{9}$$

where k_a was the equilibrium constant of adsorption and was calculated through $k_a = Q_0 \cdot b$. The enthalpy change (ΔH^0) value was obtained through the slope of the linear curve of $\ln K_a$ versus the reciprocal temperature (1/T). The values of Gibbs free-energy change (ΔG^0) and entropy change (ΔS^0) were calculated using Equations (8) and (9), respectively.

3. Results and Discussion

3.1. Adsorption of Cd(II) Ions

3.1.1. Effect of Initial Cd(II) Ion Concentrations

To examine the effect of initial Cd(II) ion concentration, different concentrations (20–160 mg L^{-1}) of Cd(II) ions were investigated. We found that if the amount of the 1,2,3,4-tetrahydropyrimidine derivative (4) in the solution is equal to 0.6 g L^{-1} and the initial Cd(II) concentration is 20 mg L^{-1}, then 98% of the Cd(II) ions are removed, whereas, if the initial concentration of the Cd(II) ions is about 160 mg L^{-1}, the amount removed falls to 79%. In addition, when the initial concentration of Cd(II)

ions ranges from 20 to 160 mg L^{-1}, the amount removed decreases progressively from 98% to 78%, respectively. Hence, the removal of Cd(II) highly depends on the concentration, especially for a higher initial concentrations. The decrease in removal efficiency may be ascribed to the fact that when the concentration of metal ions is greater, the active sites of adsorbent are surrounded by many more metal ions and, as a result, the active sites will be accommodated [35].

3.1.2. Effect of pH

To investigate the effect of pH on the removal of Cd(II) ions, many pH values (3, 4, 5, 6, 7, 8, 9, and 10) were studied at a temperature of approximately 298 ± 1 K and for Cd(II) concentrations between 20 and 160 mg L^{-1}. The contact time was set at 12 h for all experiments. The experimental results are shown in Figure 4. It was found that the adsorption efficacy of Cd(II) increased with increasing pH of the solution, and reached the maximum adsorption value at pH (6–7). Zhu et al. [36] showed similar results for their research work on the adsorption of Cd(II) and Pb(II) ions via amine-functionalized cellulose. The low metal sorption at lower pH, may be explained on the basis of active sites being protonated, resulting in a competition between H$^+$ and M^{2+} for occupancy of the binding sites [37]. The uptake of cadmium ions decreases considerably from pH 8 to 9, which can be justified by the precipitation of Cd(II) ions in an alkaline medium rich in hydroxide anions (Cd^{2+} + 2OH$^-$ → Cd(OH)$_2$) at a pH between 8 and 10.
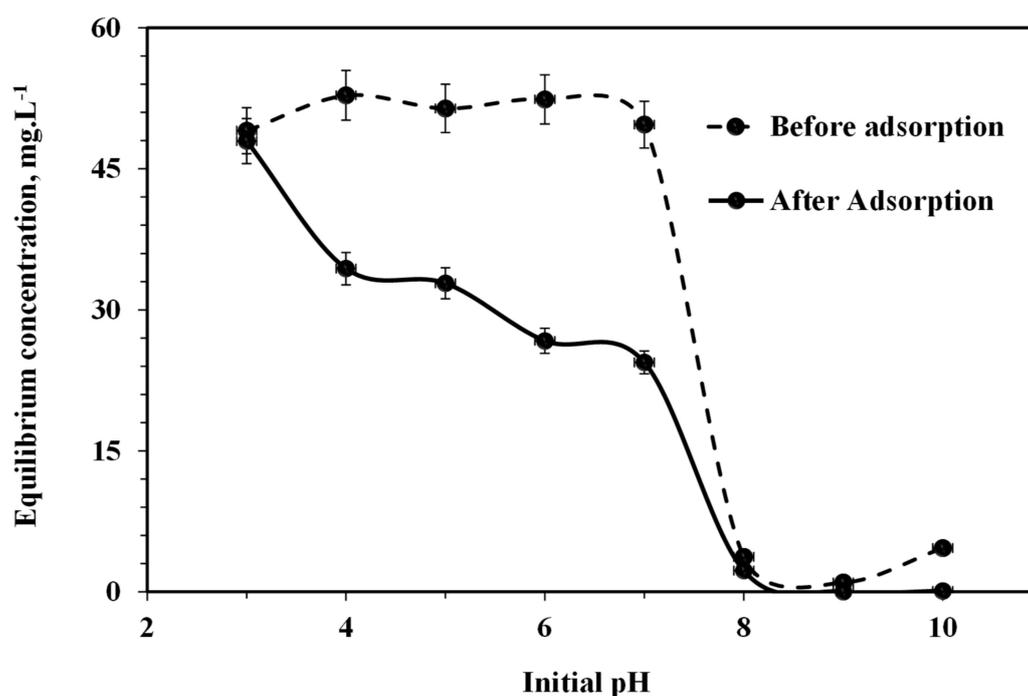

Figure 4. The initial solution pH effect on the removal of Cd(II) by 1,2,3,4-tetrahydropyrimidine at room temperature and C_0 = 52 mg/L (Dash-line without adsorbent and solid-line with adsorbent).

3.1.3. Kinetic Study

The kinetic data of the adsorption of Cd(II) ions as a function of time at 298 K are illustrated in Figure 5a,b, respectively. It shown in Figure 5a that after a rapid initial increase in adsorption q$_t$ (about 6 min), the equilibrium is reached in almost 40 min. The rapid adsorption of cadmium ions suggests that the heteroatoms (N, O) in the 1,2,3,4-tetrahydropyrimidine derivative (4) act as donor atoms to rapidly interact with the free Cd(II) ions present in the solution. Given that the coefficient of magnitude r^2 (Table 1) is the one that depends on the validity of the kinetic manners, it should be noted that for a pseudo-first-order model, the correlation coefficient was 0.9405, indicating a weak correlation, whereas the employment of a pseudo-second-order equation provided a much better correlation coefficient,

equal to 0.9977 (Table 1). The experimental and calculated values of q_e are also very close, as shown in Table 1; thereby, the pseudo-second-order kinetic equation is more appropriate for describing the adsorption kinetics behaviors of Cd(II) on the 1,2,3,4-tetrahydropyrimidine derivative (4). Zhu and colleagues [36] showed that the pseudo-second-order equation better depicts the sorption kinetics of Pb(II) and Cd(II) on amine-functionalized cellulose.
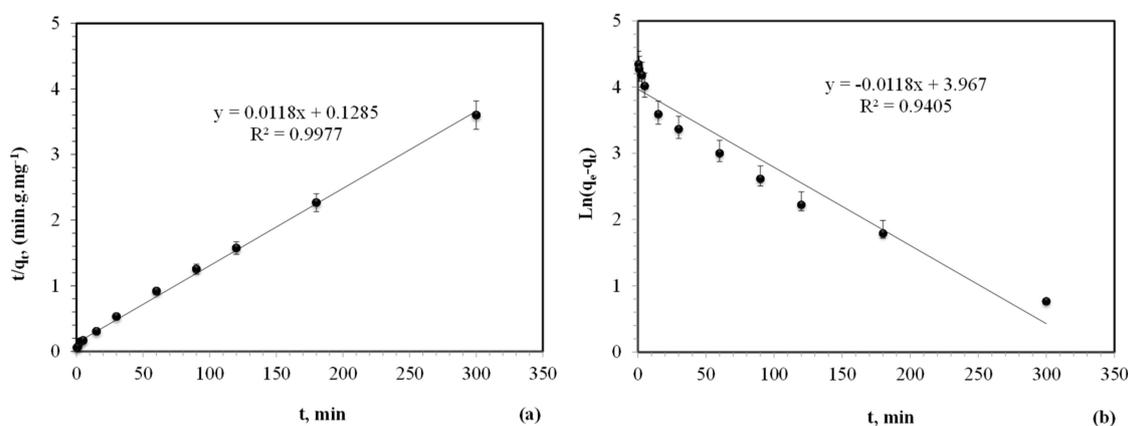

Figure 5. (**a**) Second-order and (**b**) first-order kinetic equation for adsorption of Cd(II) on 1,2,3,4-tetrahydropyrimidine at 229 K.

Table 1. Rate adsorption coefficients for first and second pseudo-order sorption kinetic models at 298 K, pH 7, and initial concentration 52 mg L^{-1}.

$t_{1/2}$	First-Order				Second-Order		
(s)	$q_{e\,(exp)}$ [a] $(mg\ g^{-1})$	k_1 (min^{-1})	$q_{e(cal)}$ [b] $(mg\ g^{-1})$	r^2	$k_2 \times 10^4$ $(g\ mg^{-1}\ min^{-1})$	$q_{e(cal)}$ [b] $(mg\ g^{-1})$	r^2
665	77	0.0118	52.83	0.9405	10.6	84.75	0.9977

[a] experimental data; [b] calculated data from models.

3.1.4. Adsorption Isotherms

The sorption studies were investigated at different temperatures (298, 308, and 318 K). The removal of Cd(II) by the 1,2,3,4-tetrahydropyrimidine derivative (4) at three different temperatures is illustrated in the Langmuir and Freundlich linear equations, as shown in Figure 6. The Langmuir and Freundlich coefficients (Q_0, b, k, n, r^2 and R_L) are listed in Table 2. With respect to the values of Q_0 and k, the effectiveness of the 1,2,3,4-tetrahydropyrimidine derivative (4) for the uptake of Cd(II) increases with increase in temperature (Table 2). It is well known that the act of increasing the temperature increases the diffusion rate of the metal ion through the outer boundary layer and into the internal pores of the adsorbent molecules, which eventually decreases the viscosity of the solution.

Given the correlation coefficients in Table 2, the experimental details better adjusted the Langmuir isotherm than the Freundlich isotherm for the adsorption of the Cd(II) ions. Therefore, the adsorption of Cd(II) ions by the 1,2,3,4-tetrahydropyrimidine derivative (4) shows the formation of a monolayer coverage of the metallic ion of cadmium with a maximum capacity of 151.16 mg g^{-1}. Reed and Matsumoto [38] investigated the removal of cadmium by a commercial activated carbon and indicated that a greater difference between n and 1 corresponds to a vast distribution of the surface bond energies. Therefore, the 1,2,3,4-tetrahydropyrimidine derivative (4) shows a large Cd(II)-surface bond energy distribution as the temperature increases.
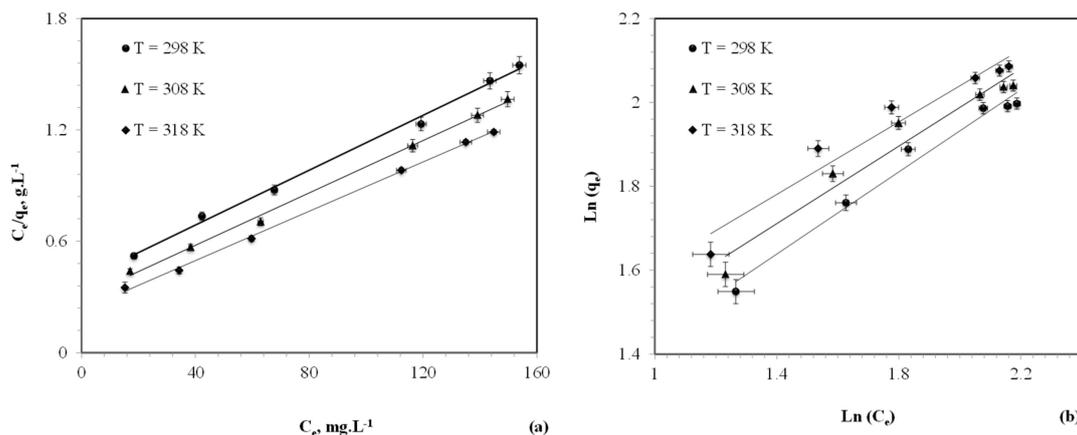
Figure 6. (**a**) Langmuir and (**b**) Freundlich equilibrium sorption isotherms for Cd(II) onto 1,2,3,4-tetrahydropyrimidine at different temperatures, pH = 7 ± 0.2.

Table 2. Effect of temperature on the values of Langmuir and Freundlich isotherm constants.

Temperature (K)	Langmuir Constants				Freundlich Constants		
	Q_0 (mg g^{-1})	b (L mg^{-1})	r^2	R_L	n	k	r^2
298	135.14	0.01896	0.9959	0.0815	2.044	8.98	0.9781
308	140.85	0.02404	0.9967	0.0679	2.164	11.58	0.9529
318	151.16	0.02959	0.9986	0.0521	2.316	14.99	0.9462

3.1.5. Thermodynamic Study

The results of the obtained thermodynamic parameters are illustrated in Table 3. The enthalpy (ΔH°) value calculated from the graph of Ln(ka) versus T^{-1} of Figure 7 exhibits the endothermic kind of the adsorption operation of Cd(II) ions, whereas the positive valor of ΔS^0 denotes the increased randomness at the 1,2,3,4-tetrahydropyrimidine derivative (4) solution interface. These obtained results are coherent with those reported by Mohaptra and Anand [39] and Mohaptra et al. [40]. The negative value of the free energy change ΔG^0 supports the spontaneous nature of the adsorption, which is proven by the R$_L$ value, and found to be less than unity. It should be noted that the value of ΔG^0 decreases when the temperature increases from 298 to 318 K, indicating that better adsorption is obtained at higher temperatures.

Table 3. Thermodynamic parameters for Cd(II) adsorption at pH = 7.

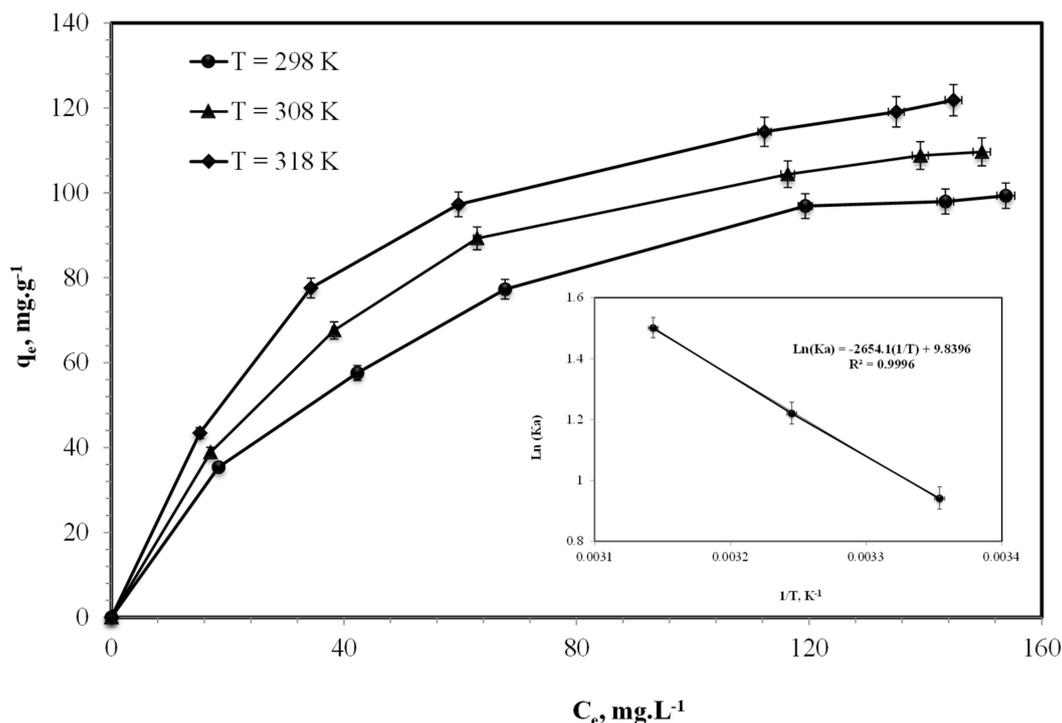| Temperature (K)	Ka	ΔG^0 (kJ mol^{-1})	ΔS^0 (kJ mol^{-1} K^{-1})	ΔH^0 (kJ mol^{-1})	r^2
298	2.562	−2.332	0.0818		
308	3.387	−3.125	0.0818	22.07	0.9996
318	4.485	−3.970	0.0818		

Figure 7. Langmuir isotherms for adsorption of Cd(II) onto 1,2,3,4-tetrahydropyrimidine at different temperatures and pH 7. The embedded figure is the plot of LnK_a against reciprocal temperature.

3.2. Mechanism of Adsorption

The uptake of cadmium ions can be controlled either by mass transfer in the liquid boundary film or by intra-particular mass transfer. The external mass transfer coefficient, β_L (m s^{-1}) of Cd(II) in the boundary film, can be evaluated using the formula [41,42]:

$$ln\left(\frac{C_t}{C_0} - \frac{1}{1 + m \cdot K_a}\right) = ln\left(\frac{m \cdot K_a}{1 + m \cdot K_a}\right) - \left(\frac{1 + m \cdot K_a}{m \cdot K_a}\right) \cdot \beta_L \cdot S_S \cdot t, \tag{10}$$

where C_t and C_0 (both in mg L^{-1}) are the respective concentrations of the metal ions at time t and zero, K_a (L g^{-1}) is a constant defined as the product of the Langmuir constants: $K_a = Q_0 \cdot$ b;m (g) is the adsorbent mass, and S_S is the adsorbent surface area (m^2 g^{-1}). A straight line in ln[($C_t/C_0 - 1/(1 + m K_a)$)] versus t plot is required to prove the reliability of the model.

The adsorbed species can also be transported from the solution to the solid phase across the intra-particle diffusion/transport procedure. The intra-particular diffusion is the limiting step in many adsorption procedures. The possibility of intra-particular diffusion was explored by the diffusion mode of Weber and Morris [43,44].

$$q_t = k_{dif} \cdot t^{1/2} + C, \tag{11}$$

where C is the intercept and k_{dif} is the intra-particle diffusion rate constant. The k_{dif} values for the tested adsorbent are calculated through the slopes of the plots (Figure 7) and described in Table 4. The validity of these models is afterward discussed.

The model of mass transfer rate based on a linear relationship between ln[($C_t/C_0 - 1/(1 + mk_a$)] and t did not provide a linear plot, demonstrating the invalidity of this model. The value of the regression coefficient is calculated from Equation (10) for the 1,2,3,4-tetrahydropyrimidine derivative (4). This means that the uptake of cadmium ions at the tested adsorbent sites is not controlled by the liquid phase mass transfer rate.

Conversely, the uptake of Cd(II) on the surface of the adsorbent may be controlled by the intra-particle diffusion kinetic model, since the values of qt are found to be linearly correlated with t$^{1/2}$

values. Besides, the regression coefficient values are equal to 0.98, indicating the applicability of this model. The intra-particle diffusion plots are shown in Figure 8. The main parameters of this model are determined and compiled in Table 4. The intercept values (i.e., *C*, Table 4) give an idea about the boundary layer thickness. The larger the intercept, the larger the boundary layer effect is.
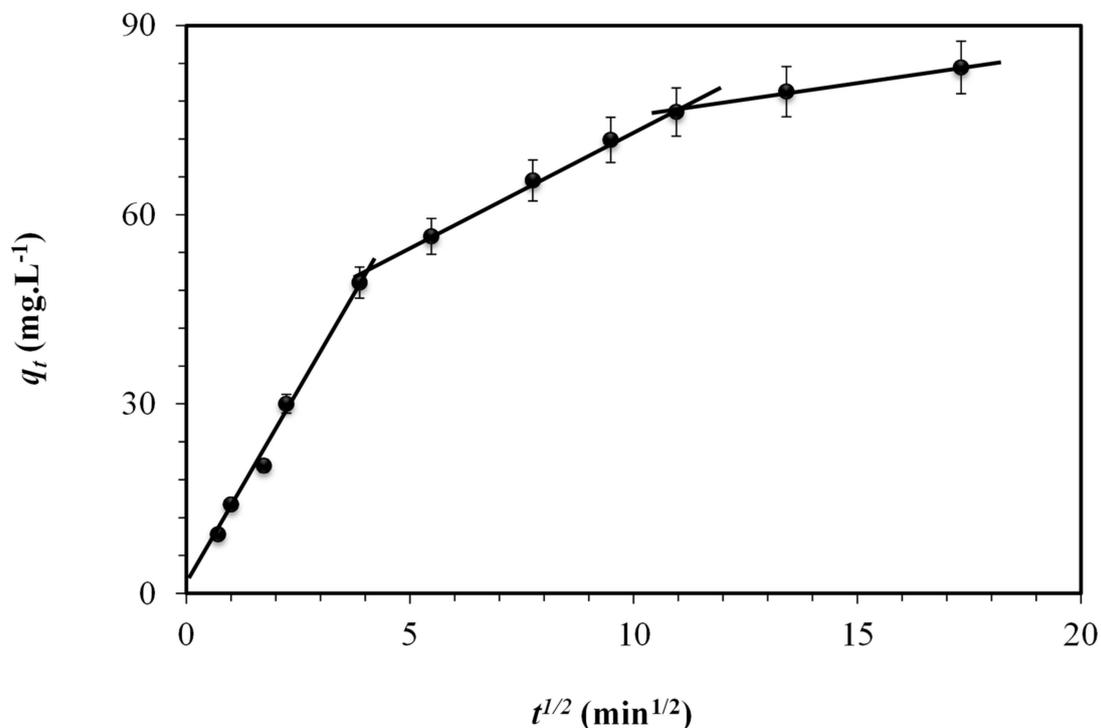

Figure 8. q_t versus t$^{1/2}$ plot for the intraparticle diffusion.

The intra-particle diffusion plot of q_t versus t$^{1/2}$ (Figure 8) shows a two-stage sorption, i.e., multi-linear [45]. The first is a sharp stage, which may have produced from the diffusion of Cd(II) through the solution to the external surface of the adsorbent and then to the surface through the boundary layer. Meantime, the second step may indicate the final equilibrium whereabouts the intra-particle diffusion begins to decelerate as a result of the lower concentration gradient of Cd(II) ions.

From the tabulated results (Table 4), it can be seen that the diffusion rate has decreased with increasing contact time due to the smaller pores accessible for diffusion, since the Cd(II) ions are formerly diffused into the internal structure of the adsorbent in the first step. This is evidenced by the smaller value of the rate parameters k_{dif1} as compared to k_{dif2}. Additionally, the constant related to the boundary layer ply (*C*) is larger in the second step, indicating a greater boundary layer effect [46].

Table 4. Kinetic parameters for the Cd(II) ions adsorption onto 1,2,3,4-tetrahydropyrimidine based on the intraparticle diffusion model.

Intraparticle Diffusion Equation Parameters								
k_{dif1}, mg/g min$^{1/2}$	C	r^2	$k_{dif\,2}$, mg/g min$^{1/2}$	C	r^2	$k_{dif\,2}$, mg/g min$^{1/2}$	C	r^2
12.58	0.56	0.9928	3.83	35.15	0.9960	1.1	64.45	0.9934

3.3. Comparison of Cd(II) Adsorption Capacity with Other Previously Reported Adsorbents

Table 5 summarizes the adsorption capacity of Cd(II) ions by the 1,2,3,4-tetrahydropyrimidine derivative (4) and other alternative adsorbents as reported in the literature. The 1,2,3,4-tetrahydropyrimidine

derivative (4) described in this work presents a better adsorption performance and shows a higher adsorption capacity for Cd(II) than other adsorbents reported in the literature.

Table 5. Comparison of 1,2,3,4-tetrahydropyrimidine adsorption capacity with some adsorbents for cadmium (II).

Adsorbent	q_e (mg g^{-1})	Temp. (K)	Ref.
C,N-pyridylpyrazole	4.8	298	[47]
Gallic acid	6.09	298	[48]
3-Aminopropytriethoxysilane	14.1	323	[49]
Chitosan/cotton fibers	15.74	298	[50]
Melamine-based NH$_2$ dendrimer	71.1	323	[49]
Spirodela polyrhiza	36	298	[51]
Pyrazol-3-ylimine	74.89	298	[52]
CMJF$_{MH}$	88	298	[53]
PEI/SA-MCCMV	139.47	298	[36]
Present Work	135.14	298	-
Present Work	151.16	318	-

4. Conclusions

This research work presented the 1,2,3,4-tetrahydropyrimidine derivative as an effective and rapid absorption of Cd(II) ions from aqueous solutions. The equilibrium data were fitted to the Freundlich and Langmuir isothermal models. At a pH value of 6–7 at 328 K, an adsorption capacity of cadmium ions of approximately 151.16 mg g^{-1} was obtained. Both pH and temperature are critical parameters for the extension of Cd(II) uptake. Furthermore, the suitability of the kinetic models for the adsorption of Cd(II) ions on the 1,2,3,4-tetrahydropyrimidine derivative was also discussed. The kinetic measurement of the adsorption process of Cd(II) ions is considered to follow a pseudo-second-order rate law. The evaluated thermodynamic parameters indicate that the adsorption process of Cd(II) ions on the milled goethite is spontaneous and endothermic.

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