Al-Kitab Journal for Pure Sciences (2025); 9(2):169-180.
https://doi.org/10.32441/kjps.09.02.p11

Al-Kitab Journal for Pure Sciences
ISSN: 2617-1260 (print), 2617-8141(online)

https://isnra.net/index.php/kjps

Synthesis, Characterization, and CO2 Capture Application of Cu(II)-paracetamol complex

Mohanad Ali Sultan

Department of Chemical Engineering, College of Engineering, University of Diyala, Baqubah, Iraq

*Corresponding Author: maalazzawi85@uodiyala.edu.iq

Citation: Sultan MA. Synthesis, Characterization, and CO2 Capture Application of Cu(II)-paracetamol complex. Al-Kitab J. Pure Sci. [Internet]. 2025 Sep. 07;9(2):169-180. DOI: https://doi.org/10.32441/kjps.09.02.p11

Keywords: Cu(II), Paracetamol, CO_2 Capture, Metal Complexes , Tridentate Ligand.

Article History

Received	26 Jun. 2025
Accepted	31 Jul. 2025
Available online	08 Sep. 2025

Abstract:

A cu(II)-paracetamol complex was synthesized and characterized using UV-Vis and FTIR spectroscopy and melting point analysis. The ligand paracetamol acted as a tridentate chelating agent, coordinating through the hydroxyl, carbonyl, and amine groups. The complex was found to be more soluble in DMSO. Job's method of continuous variation suggested a 1:2 metal-to-ligand stoichiometry. The synthesized Cu(II) complex was evaluated for CO_2 adsorption performance, demonstrating promising uptake capacity due to the strong affinity of the metal center for CO_2 molecules.

Keywords: Cu(II), Paracetamol, CO_2 Capture, Metal Complexes, Tridentate Ligand.

تحضير، توصيف، وتطبيق احتجاز ثاني أكسيد الكربون لمعقد النحاس-باراسيتمول

الخلاصة:

تم تحضير وتوصيف معقد-Cu(II) باراسيتامول باستخدام أطياف الأشعة فوق البنفسجية-المرئية (UV-Vis) وتقنية الأشعة تحت الحمراء (FTIR) بالإضافة إلى تحليل نقطة الانصهار. عمل الباراسيتامول كـ ليغند ثلاثي السن، منسقاً من خلال مجموعات الهيدروكسيل والكربونيل والأمين. وُجد أن المعقد أكثر ذوبانية في DMSO. أظهرت طريقة جوب للتغير المستمر أن نسبة المعدن إلى الليغند هي ١:٢. تم تقييم المعقد المحضر من Cu(II) من حيث أدائه في امتصاص غاز ثاني أكسيد الكربون، حيث أظهر قدرة امتصاص واعدة بسبب قوة التآلف العالية بين مركز المعدن وجزيئات CO_2.

الكلمات المفتاحية: Cu(II)، باراسيتامول، احتجاز ثاني أكسيد الكربون، المعقدات الفلزية، ليغند ثلاثي السن.

1. Introduction:

Paracetamol (acetaminophen) is a commonly used analgesic and antipyretic drug that has also gained attention in coordination chemistry [1] [2]. Paracetamol exhibits important ligand properties due to the presence of hydroxyl (-OH), amine ($-NH_2$), and carbonyl (C=O) groups, making it suitable for coordination with transition metals [3] [4]. These groups act as donor sites in chelation, forming stable complexes with various metal ions.

Copper(II) ions are particularly valuable in coordination chemistry due to their flexible geometry, strong Lewis acidity, and redox activity. Cu(II) complexes have shown monumental applications in catalysis, antibacterial agents, and environmental treatment [5]. When coordinated with multidentate ligands such as paracetamol, copper ions often adopt square planar or distorted octahedral geometries, depending on ligand field strength [6].

Copper(II) complexes of various ligands have demonstrated wide biology and catalytic applications due to the favorable redox behavior of cu(II) ions. Despite studies on Cu(II)-paracetamol complexes in biomedical and catalytic areas, their potential role in environmental applications- especially CO_2 capture- remains largely unexplored. This represents a critical research gap, especially given the global need for sustainable and cost-effective carbon dioxide sequestration technology [7].

Traditional adsorbents such as zeolites, activated carbon, and metal-organic frameworks (MOFs) are widely studied for CO_2 capture. However, challenges such as high cost, synthetic complexity, or recovery difficulty limit their broader usages [8] [9] [10]. Recent literature has shown the importance of exploring novel coordination complexes as functional CO_2 adsorbents. The strong Lewis acidity of Cu(II) and the formation of a polar surface upon complexation make such materials promising for binding CO_2 through physisorption or chemisorption mechanisms [11] [12][13].

The objective of this study is to synthesize and characterize a Cu(II)-paracetamol complex, investigate its coordination manner, and evaluate its performance in CO_2 capture. A schematic representation of the expected coordination structure will later be provided in the Discussion section to clarify the binding mode between copper and paracetamol. The importance of this work demonstrates a simple, accessible, and functional coordination complex stemming from a pharmaceutical ligand for environmental CO_2 capture under mild conditions.

2. Material and methods:

Pure paracetamol ($C_8H_9NO_2$, 99% purity), melting point:(169°C) was obtained from Kendy Pharmaceuticals, $Cu(NO_3)_2.6H_2O$ analytical grade, methanol, and distilled water were used as solvents. The copper complex was synthesized by mixing 0.01 mol of $Cu(NO_3)_2.6H_2O$ dissolved in 100 ml of distilled water and 0.02 of paracetamol dissolved in 100 ml of methanol. The reaction mixture was mixed and stirred for 1 hour at room temperature (~25°C) and subsequently heated at 60 °C for 2 hours on a hot plate until all the solution was evaporated. A greenish-dark precipitate was formed, filtered using a Bucher funnel, and dried at ambient temperature. The obtained complex was characterized for thermal stability, color, and spectroscopic signatures [14].

FTIR spectra were recorded in the range of 400 -4000 cm^{-1} using KBr pellets (1:100 sample-to-KBr ratio). Spectra were collected for both the free ligand and the synthesized complex to identify shifts in functional group frequencies due to metal coordination. Additionally, UV-Visible spectra were obtained in the range of 200 -800 nm using methanol as solvent. Absorbance changes between free ligand and complex solutions were evaluated to confirm electronic transitions and coordination [15] [16]. Moreover, the Job's method of continuous variation was used to determine metal-to-ligand stoichiometry, where absorbance values at a fixed wavelength were plotted against mole fractions of paracetamol [17]. Gravimetric CO_2 adsorption experiments were conducted within a temperature range from 25 to 60 °C under 1 atm pressure, in which adsorbent mass and exposure time were kept constant, and uptake values were calculated in mmol/g. Additionally, as the entire process was done in the solid phase, PH control was not necessary.

3. Results:

The coordination of paracetamol with the Cu(II) ion was elucidated through Fourier Transform Infrared Spectroscopy (FTIR) and Ultraviolet-Visible (UV-Vis) Spectroscopy, which are key techniques for confirming metal-ligand interactions and electronic transitions in coordination compounds [18]. Moreover, the Cu(II)-paracetamol complex showed observable CO_2 adsorption performance under room and increased temperatures. At 25 ^{0}C and 1 atm, the complex demonstrated a CO_2 uptake of 1.22 mmol/g, indicating moderate affinity toward CO_2. As the temperature increased, the adsorption capacity decreased to 0.95 mmol/g at 40 ^{0}C and 0.59 mmol/g at 60 ^{0}C, compatible with the exothermic nature of physisorption. The adsorption manner followed the Langmuir isotherm model, indicating monolayer surface coverage and confirming physical adsorption as the main mechanism [19] [20] [21]. The trend shows that the CO_2 capture is favorably achieved at lower temperatures. Compared to the standard adsorbents such as activated carbon and zeolites, the Cu(II)-paracetamol performs within a suitable range, highlighting its importance as an easy synthesis and a cost-effective material for CO_2 capture applications.

4. Discussion

The FTIR spectrum of free paracetamol revealed characteristic vibrational modes assigned to its functional groups for its structural identity and purity. The broad band around 3325 cm^{-1} is assigned to O-H stretching, which is typically appears in this region due to hydrogen bonding Additionally , a distinct sharp band at 3163 cm^{-1} corresponds to N-H stretching of the amine group, confirming the presence of an acetamide moiety in the molecule.

Another prominent peak observed at 1650 cm^{-1} is attributed to C=O (carbonyl) stretching of the amide functionality. This band is generally strong and sharp, supporting the presence of a conjugated amide system. The C-N bending and N-H bending vibrations typically appear between 1500-1580 cm^{-1} and indeed several medium-intensity bands are seen in that region, reinforcing the assignment of an acetamide structure.

Furthermore, peaks observed in the region of 1240-1020 cm^{-1} are consistence with C-O stretching vibrations from the phenolic group, and the out-of-plane C-H bending of the armoctic ring appears in the 750-840 cm^{-1} range.

These spectral features collectively confirm the presence of hydroxyl , amide, and aromatic functionalities in the paracetamol molecule. **Figure 1** shows the FITR spectrum of free paracetamol , clearly indicating all characteristic absorption bands discussed.

Upon complexation with Cu(II), significant shifts and changes in these absorption bands were observed in the FTIR spectrum of paracetamol, indicating coordination through multiple donor sites. Specifically, the O-H stretching band was shifted from 3325 cm^{-1} to approximately 3562 cm^{-1} in the complex, indicating involvement of the phenolic –OH group in direct coordination to the metal center, albeit without full deprotonation. Furthermore, the N-H stretching band at 3163 cm^{-1} , which was clearly visible in the free paracetamol spectrum, completely disappeared from the spectrum of the Cu(II) complex. This disappearance supports the coordination of the amide nitrogen to the metal center via the lone pair donation, suggesting chelation through the nitrogen atom.

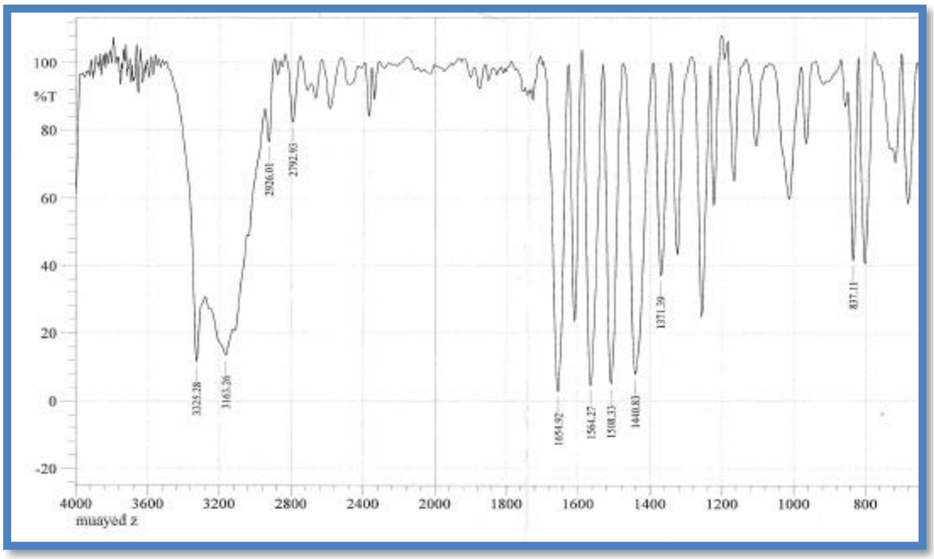

Figure 1: FTIR spectrum of pure paracetamol, showing characteristic absorption bands of functional groups present in the molecule

The C=O band, typically observed at 1650 cm^{-1}, was significantly shifted to a broader, less intensity region between 1614-1548 cm^{-1}. This red shift in the carbonyl vibration is characteristic of coordination via the carbonyl oxygen, which weakens the C=O bond due to electron delocalization toward the metal ion. Such behavior is well-known in the metal-amide complexes binding modes. Additional spectral changes were observed in the low-frequency region (<600 cm^{-1}) where new bands emerged that were absence in the spectrum of free paracetamol. These are assigned to M-O and M-N stretching vibrations, further confirming the formation of a metal-ligand coordination network.

Altogether, these spectral changes- namely the shift or disappearance of O-H, N-H, and C=O bands,and the appearance of metal-ligand vibrational modes - strongly confirm that paracetamol behaves as a tridentate ligand, binding through its hydroxyl oxygen, amide nitrogen, and carbonyl oxygen atoms. This coordination configuration forms a stable chelate with Cu(II), likely resulting in a six-membered chelate ring. Figure 2 presents the FTIR spectrum of the Cu(II)-paracetamol complex, clearly showing the discussed changes and confirming successful complex formation.

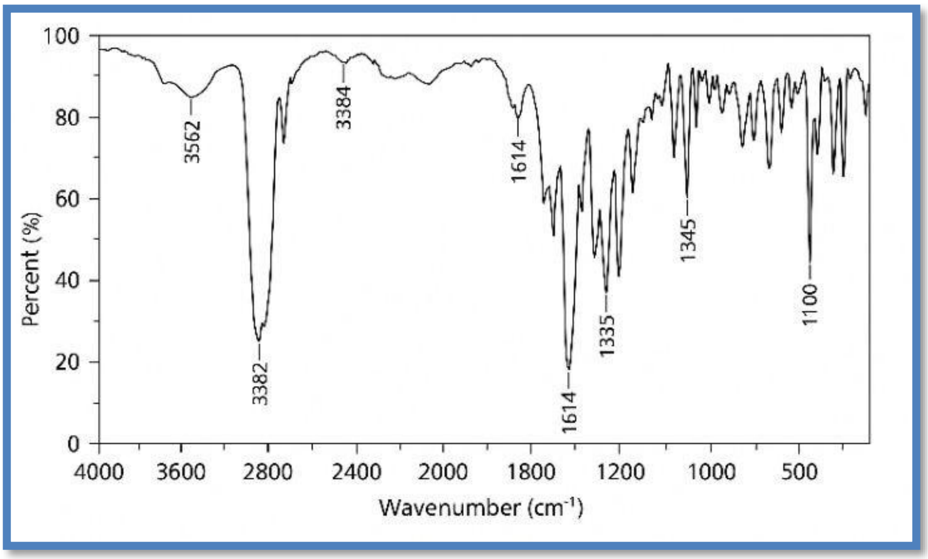

Figure 2:FTIR spectrum of pure Cu(II)-paracetamol complex, showing characteristic absorption bands. Key peaks indicate the presence of functional groups involved in complexation.

UV-Vis absorption spectrum of the free paracetamol ligand exhibited a prominent peak around ~243 nm, shown in Figure 3, which is associated with π → π* transitions of the aromatic ring system. These transition are characteristic of conjugated systems and provide evidence of the electronic configuration and aromatic character of the ligand. The band reflects the presence of delocalized π electrons in the phenyl ring of paracetamol and is often used as a fingerprint region for aromatic compounds.

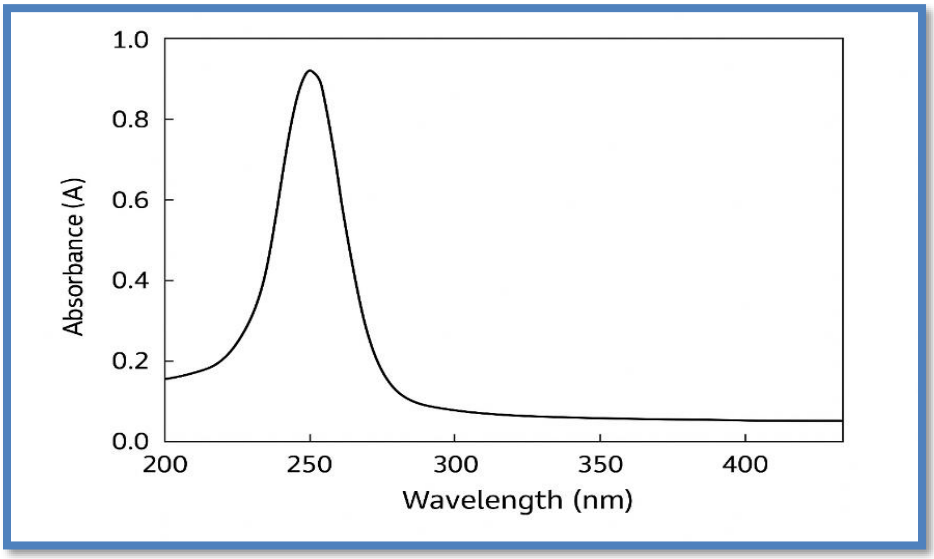

Figure 3: UV-Visible absorption spectrum of free paracetamol.

However, upon complexation with Cu(II), the absorption maximum (λ max) was red-shifted to approximately 340 nm, indicating a change in the electronic environment of the ligand due to metal coordination as depicted in Figure 4. This bathochromic shift is characteristic of n → π* transitions and ligand-to-metal charge transfer (LMCT) interactions, suggesting a strong interaction between the lone pair electrons (particularly on oxygen and nitrogen atoms) and the Cu(II) metal center. Such transitions are indicative of delocalization of electron density across the metal-ligand framework, which is common in chelated systems involving transition metals. The presence of a d-d transition band observed near 580 nm was also observed in the visible region, often contributing to the distinctive greenish coloration of the complex. These electronic transitions are consistent with a distorted octahedral or square planar geometry, commonly adopted by Cu(II) complexes, depending on the ligand field strength and donor set.

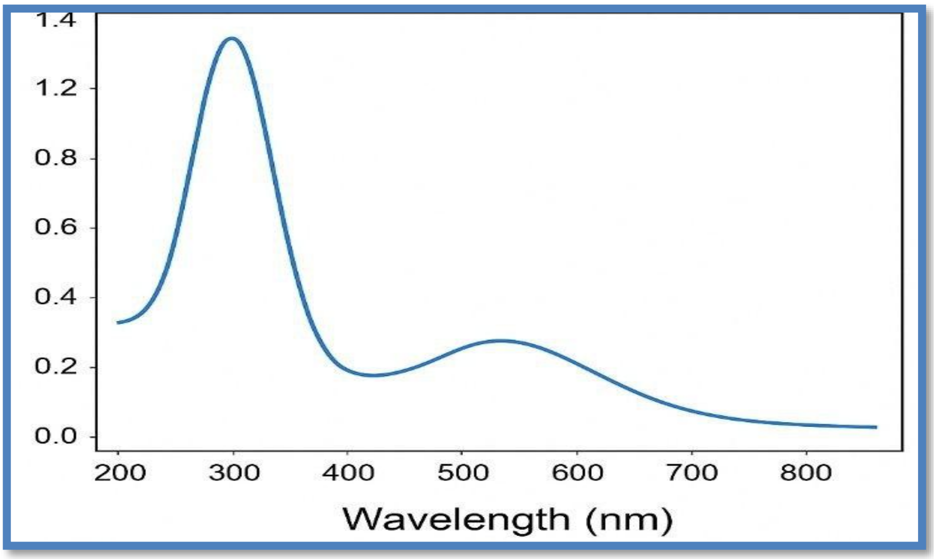

Figure 4: UV-Visible absorption spectrum of the copper-paracetamol complex recorded in the range of 200-800 nm

The plot of continuous variations (Job's method) provides important insights into the stoichiometry and complexation behavior between copper (II) and paracetamol in solution. The absorbance is plotted against the mole fraction of paracetamol to determine the binding ratio between the central ion and the ligand shown in **Figure 5**.

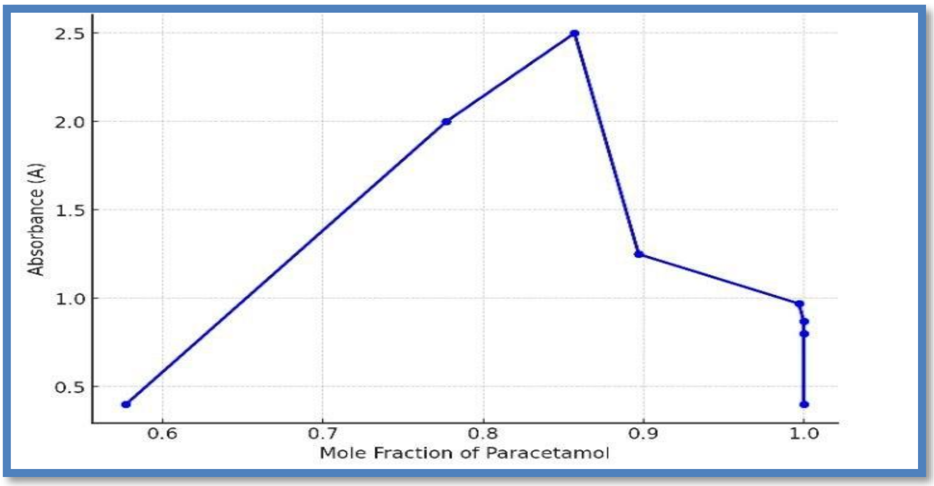

Figure 5: Jon's method plot showing the variation in absorbance of the Cu(II)-paracetamol complex with mole fraction of paracetamol, indicating a 1:2 metal-to-ligand stoichiometry at maximum absorbance (0.857 mole fraction)

The curve in **Figure 5** shows a distinct profile characterized by a gradual increase in absorbance as the mole fraction of paracetamol increases, reaching a maximum at about 0.857 mole fraction, followed by a successive decrease. The maximum absorbance peak is associated with the composition at which the molar ratio of approximately 1:2 metal-to-ligand ratio, suggesting that each copper ion binds with two molecular units of the ligand. Such stoichiometric data are consistent with prior works on Cu(II)-paracetamol complex **[22] [23],** and the proposed coordination environment is further supported by FTIR and UV-Visible. Spectroscopic findings. The ligand-to-metal ratio indicates a strong interaction between the phenolic, amide, and carboxylate groups of paracetamol, possibly forming an octahedral coordination environment. To support the Job's plot data, **Figure 6** illustrates a schematic bonding diagram of the proposed Cu-paracetamol complex, confirming the tridentate configuration. This structural presentation is crucial for correlating spectroscopic changes with the complex geometry.

The decline in absorbance beyond the 0.857 mole fraction indicates that excess paracetamol does not contribute to further complex formation. Instead, it may give rise to ligand saturation. This means that free paracetamol stays unbound in solution and does not produce the UV-Visible absorbing complex. Therefore, the overall absorbance is decreased due to the dilution of the complex concentration.

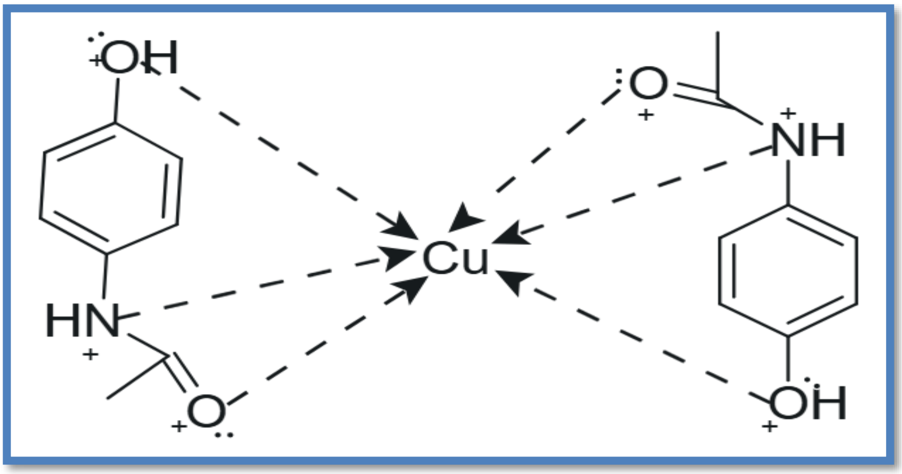

Figure 6: Proposed structure of the Cu(II)-paracetamol complex showing tridentate coordination by each paracetamol ligand through the phenolic-OH, amide nitrogen, and carbonyl oxygen, resulting in an octahedral geometry around the central Cu^{2+} ion

The adsorption measurements were done under 1 atm pressure for 60 minutes using 100 mg of the complex in a sealed chamber. The complex exhibited CO_2 uptake of 1.22 mmol/g 25°C and at 60 °C, the uptake values decreased to 0.59 mmol/g as shown in **Table 1**. The manner is consistent with the Langmuir model, which is expressed as $qe = \frac{qmax\ KL\ Ce}{1+KL\ Ce}$ **[24] [25].**

Where:

q_e is the amount of adsorbate at equilibrium (mmol/g)

q_{max} is the maximum adsorption capacity (mg/g)

Ce is the equilibrium concentration of adsorbate (mg/L)

and

KL is the Langmuir constant related to the affinity of binding sites (L/mg)

Table 1: CO_2 adsorption capacity of the Cu(II)-paracetamol complex at different temperatures under 1 atm pressure.

Temperature	Pressure	CO_2 Uptake (mmol/g)
25 ^{0}C	1 atm	1.22
30 ^{0}C	1 atm	1.13
35 ^{0}C	1 atm	1.04
40 ^{0}C	1 atm	0.95
45 ^{0}C	1 atm	0.86
50 ^{0}C	1 atm	0.77
55 ^{0}C	1 atm	0.68
60 ^{0}C	1 atm	0.59

To demonstrate the thermal behavior of CO_2 adsorption on the complex surface, an Arrhenius-type plot of ln(qe) versus 1/T (K^{-1}) was constructed using the experimental uptake values at different temperatures. A good linear relationship was noticed, suggesting the temperature dependence of adsorption follows the Arrhenius equation. The slope of the line was used to determine the adsorption energy, which was found to be **-16.89kJ/mol**. This negative value confirms the exothermic nature of the adsorption process and is unique to physisorption, where a relatively weak van der Waals interaction is the main force between the adsorbate CO_2 and the adsorbent surface, as shown in **Figure 7**.

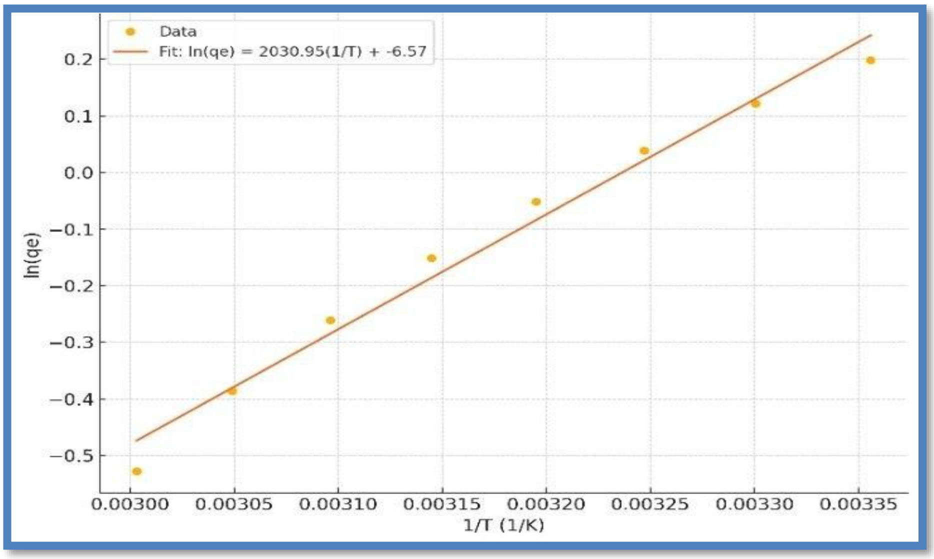

Figure 7: Arrhenius plot of ln(q_e) vs. 1/T for CO_2 Adsorption onto the complex

The Cu(II)-paracetamol complex demonstrated a CO_2 adsorption capacity of 1.22 mmol/g at 25 °C and 1 atmosphere, which is a significant result when compared with the class of molecular coordination complexes. This uptake indicates that the synthesized material possesses a moderately high affinity for CO_2 under ambient conditions, suggesting favorable thermodynamic and kinetic interaction between the gas molecules and the adsorbent. From a coordination chemistry perspective, the Cu(II) center acts as a Lewis acid with an open coordination site or labile positions in the ligand field. The adsorption mechanism is dominated by physisorption, likely driven by dipole-quadruple interaction between the polar Cu(II) center and linear CO_2 molecules. The presence of functional groups such as hydroxyl(-OH), carbonyl (C=O), and amine ($-NH_2$) in the paracetamol ligand contributes additional Lewis basic sites, facilitating localized CO_2 adsorption via hydrogen bonding or acid-base. Furthermore, the relatively high uptake at 25 °C- where adsorption is typically thermodynamic favored- is consistent with physisorption behavior. The result also indicates that no significant steric hindrance occurs with the complex structure that would otherwise inhibit CO_2 accessibility to active sites. It is likely that the complex forms a supramolecular network or aggregates that retain free volume or interstitial voids, providing an accessible microenvironment for gas diffusion and retention [26]. In terms of performance benchmarking, the value of 1.22 mmol/g places this material in the same operational range as many non-porous adsorbents and functionalized organic compounds seen in Table 2. While it is not as high as metal-organic frameworks (MOFs), which often exceed 4.4 mmol/ g under similar conditions, it offers distinct advantages in terms of synthesis simplicity, stability in ambient environments, and potential biodegradability, which are crucial for low-cost and CO_2 management systems.

Table 2: Comparison of CO_2 uptake capacities at 25 ^{0}C for various adsorbent materials

Materials type	**Uptake at 25 °C mmol/g**
Amine-functionalized silica	1.0-3.5
Zeolites	2.5-3.0
MOFs (e.g, HKUST-1)	4.5-6.0
Activate carbon	0.8-2.0
Cu(II)-paracetamol complex	**~1.22**

5. Conclusions

This study successfully synthesized a cu(II)-paracetamol complex, characterized by FTIR, UV-Vis spectroscopy, and stoichiometry analysis. The spectral data confirmed coordination through the hydroxyl , amine, and carbonyl groups of paracetmol, forming a tridentate ligand. UV.Vis analysis showed red-shifted absorption, indicating metal-ligand interactions. The complex exhibited a CO_2 uptake capacity of ~1.22 mmol/g under ambient conditions, suggesting potential as a cost-effective and environmental friendly CO_2 capture material. These results demonstrate the dual utility of the complex in both pharmaceutical coordination chemistry and environmental applications.

6. References

[1] Lawal A, Obaleye JA. Synthesis, characterization and antibacterial activity of aspirin and paracetamol metal complexes. Biokemistri. 2007;19(1):17–23.

[2] Adadey SM, Sarfo JK. Copper-paracetamol complexes: promising lead antibacterial drug candidates. Afr J Pure Appl Chem. 2016;10(5):56–62.

[3] Osowole AA, Ojo BO. Synthesis and characterization of mixed ligand transition metal complexes of paracetamol and vanillin. Asian J Pharm Clin Res. 2014;7(3):145–9.

[4] Chui SSY, Lo SMF, Charmant JPH, Orpen AG, Williams ID. A chemically functionalizable nanoporous material $[Cu_3(TMA)_2(H_2O)_3]_n$. Science. 1999;283(5405):1148–50.

[5] Kulkarni PP, Jadhav PD, Patil VS, Deshmukh CD. Synthesis, characterization and antimicrobial studies of Cu(II) complexes with biologically active ligands. J Chem Pharm Res. 2012;4(1):726–31.

[6] El-Sherif AA, Ali H, Ahmed SM. Spectroscopic studies and biological activity of novel metal complexes of paracetamol. Spectrochim Acta A Mol Biomol Spectrosc. 2009;72(4):897–902.

[7] Mohapatra S, Parida KM. A review on CuO-based composite materials for CO_2 capture and catalytic conversion. RSC Adv. 2016;6(84):80047–68.

[8] Sumida K, Rogow DL, Mason JA, McDonald TM, Bloch ED, Herm ZR, et al. Carbon dioxide capture in metal-organic frameworks. Chem Rev. 2012;112(2):724–81.

[9] Wang Q, Luo J, Zhong Z, Borgna A. CO_2 capture by solid adsorbents and their applications: current status and new trends. Energy Environ Sci. 2011;4(1):42–55.

[10] Nakamoto K. Infrared and Raman Spectra of Inorganic and Coordination Compounds. 6th ed. Hoboken (NJ): Wiley; 2009.

[11] Lever ABP. Inorganic Electronic Spectroscopy. 2nd ed. Amsterdam: Elsevier; 1984.

[12] Raganati F, Liguori B, Ammendola P. Adsorption of carbon dioxide on solid sorbents: a review. Energy Fuels. 2021;35(1):1287–1314.

[13] Wang J, Luo J, Zheng Y, Wang S. Recent advances in solid sorbents for CO_2 capture: a review. J Clean Prod. 2017;161:821–839.

[14] Sultan MA, Karim AE, Kandory A, Al-Metwali A. Synthesis and characterization of Al(III) complex with paracetamol. Int J Pharm Qual Assur. 2020;10(1):156–9.

[15] Structure-Properties Relationship of Cu(II)–Paracetamol Based Complex: a theoretical and spectroscopic study. Napdd Intl J Pharm Drug Deliv Tech. c2021.

[16] Synthesis and characterization of metal complexes of Mg(II) and Cu(II) ions with N-(4-hydroxyphenyl)acetamide. J SSRR. 2025;22 Jan.

[17] Rose NJ, Drago RS. Generalization of the Job method of continuous variation for complex stoichiometry. J Am Chem Soc. 1959;81(24):6138–41.

[18] El-Shahawy MA, et al. Synthesis and characterization of Fe(II), Cu(II), Zn(II) complexes with paracetamol. Korea Scie. c2022.

[19] Adsorption of paracetamol onto activated carbon derived from sawdust. Sustainability. 2023;15(3):2516.

[20] Removal and adsorption characteristics of paracetamol using hemp-derived activated carbon: Langmuir & Freundlich modelling. Environ Eng Res. 2022;37(4):357–368.

[21] Adsorption mechanisms of paracetamol on graphene-based nanomaterials: experimental and DFT insights. Front Carbon Res. 2024.

[22] Kulkarni PP, Jadhav PD, Patil VS, Deshmukh CD. Synthesis, characterization and antimicrobial studies of Cu(II) complexes with biologically active ligands. J Chem Pharm Res. 2012;4(1):726–731.

[23] Sarkar S, Das A, Dutta C. Cu(II) complex of paracetamol: Structure and spectroscopic characterization. Polyhedron. 2020;175:114159.

[24] STM and DFT studies of CO_2 adsorption on Cu surfaces indicate weak, physisorptive interactions (~15-20 kJ/mol). arXiv. 2018.

[25] Ion-imprinted strategy for Cu-based adsorbents: application for CO_2 capture and catalytic compatibility. J Hazard Mater. 2025.

[26] A new tridentate Schiff base Cu(II) complex: synthesis, FTIR, UV-Vis and single-crystal analysis. J Inorg Organomet Polym. 2013;23:1015-1025.