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Spectral Interpretation of Dye Adsorption on Activated Carbons

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Abstract

Activated carbons can remove dissolved dyes through interactions governed by accessible porosity, surface chemistry and solution conditions. This review explains how Fourier-transform infrared (FTIR) spectroscopy, ultraviolet–visible (UV–Vis) analysis, equilibrium isotherms and kinetic models contribute to interpretation of adsorption. FTIR changes may suggest altered functional-group environments but do not uniquely establish a binding mechanism. Calibrated UV–Vis measurements estimate residual dissolved dye concentration when matrix effects and alternative losses are controlled. Langmuir and Freundlich equations describe equilibrium behavior, whereas pseudo-first-order and pseudo-second-order models empirically describe uptake kinetics. A high coefficient of determination alone does not establish monolayer coverage, equivalent sites or chemisorption. Reliable interpretation requires controls, reproducibility, uncertainty analysis and complementary characterization. No raw spectra, measured capacities or fitted constants are reported; the figures are conceptual schematics or reproduced from open-access literature with attribution.

Keywords: *activated carbon; dye adsorption; FTIR; UV–Vis spectroscopy; adsorption isotherms; kinetic modeling.*

1. Introduction

Adsorption is accumulation at an interface. In an aqueous dye–carbon system, the dye is the adsorbate and the solid is the adsorbent. Adsorption depends on pore accessibility, surface chemistry, dye properties and solution conditions. Activated carbon should be distinguished from a merely carbonized precursor: activation and characterization must be documented before claims about developed porosity are made. No isolated spectral band or fitted equation explains every dye–carbon system [1]. [9,12]

2. Preparation and characterization

Report precursor identity, pretreatment, particle size, carbonization atmosphere, heating rate, temperature and residence time. Describe activation separately, including physical or chemical treatment conditions and reagent-to-precursor ratio where relevant. Washing, drying, storage and dry-mass basis also require documentation. A single temperature range is not a universal activation protocol [1]. [12]

Complementary characterization can assess accessible surface area, pore-size distribution, surface composition and pH-dependent surface charge. FTIR does not measure surface area, establish microporosity or count adsorption sites. Relate preparation to performance using multiple types of evidence [1,2]. [10]

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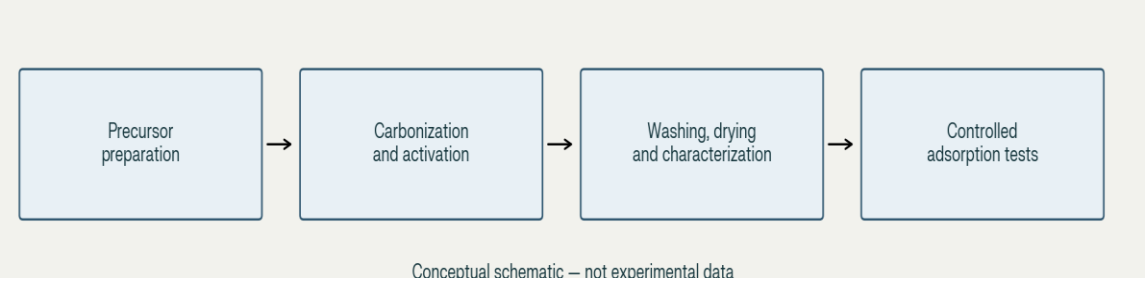


Figure 1. General preparation and testing workflow. Conditions must be documented for the actual material.

Gas-physisorption measurements provide information on surface area and pore-size distribution that cannot be obtained from FTIR alone. The IUPAC technical report provides standardized terminology and methodological guidance for interpreting such measurements. Consequently, spectral assignments should be discussed alongside independently established textural properties rather than treated as evidence of microporosity [10].

3. FTIR spectroscopy

FTIR measures infrared absorption associated with molecular vibrations. Carbon spectra often contain broad, overlapping bands; assignments are tentative unless supported by suitable reference spectra and complementary measurements. Drying, sample loading, sampling mode, ATR contact and baseline or normalization procedures affect apparent intensities [2].

Table 1. Illustrative infrared regions, not measured peak positions for a sample in this review [2].

Approximate region (cm^{-1})	**Possible contribution**	**Interpretive caution**
3600–3200	O–H stretching: hydroxyl groups and/or water	Changes are not unique evidence of dye–surface hydrogen bonding.
1750–1650	C=O stretching in suitable groups	Position varies with chemical environment; overlap is possible.
1650–1500	Aromatic skeletal vibrations and overlapping modes	Water bending near 1640 cm^{-1} and dye bands may overlap.
1300–1000	C–O-related and other fingerprint-region modes	A band does not uniquely identify one surface functionality.

Compare unloaded carbon, dye reference material, recovered loaded carbon and relevant blanks under consistent preparation and acquisition conditions. Reproducible changes may support altered local environments but do not independently prove covalent bonding or chemisorption. Dye-associated bands on a recovered solid may indicate retention of dye or related species; they do not exclude simultaneous degradation or retention of transformation products [1,2]. [9]

Genuine literature examples illustrate typical spectral changes. Figure 3 reproduces open-access FTIR spectra of Rumex abyssinicus-derived activated carbon before and after adsorption of malachite green [6]. Before adsorption, broad O–H bands appear near 3500–3290 cm^{-1}, with features attributed to carboxyl, C=O/C=C, aromatic C=C (~1543 cm^{-1}) and C–O modes. After adsorption, several peaks diminish, shift or vanish (including loss of certain O–H and residual activating-agent features), consistent with involvement of oxygen-containing groups and aromatic domains. Similar comparisons for other dyes (e.g., AO7 on coffee-ground carbon [7], RBBR on hybrid-modified carbon [8]) commonly show intensity changes or shifts in the 3600–3200, 1700–1500 and fingerprint regions without uniquely proving a single binding mode.

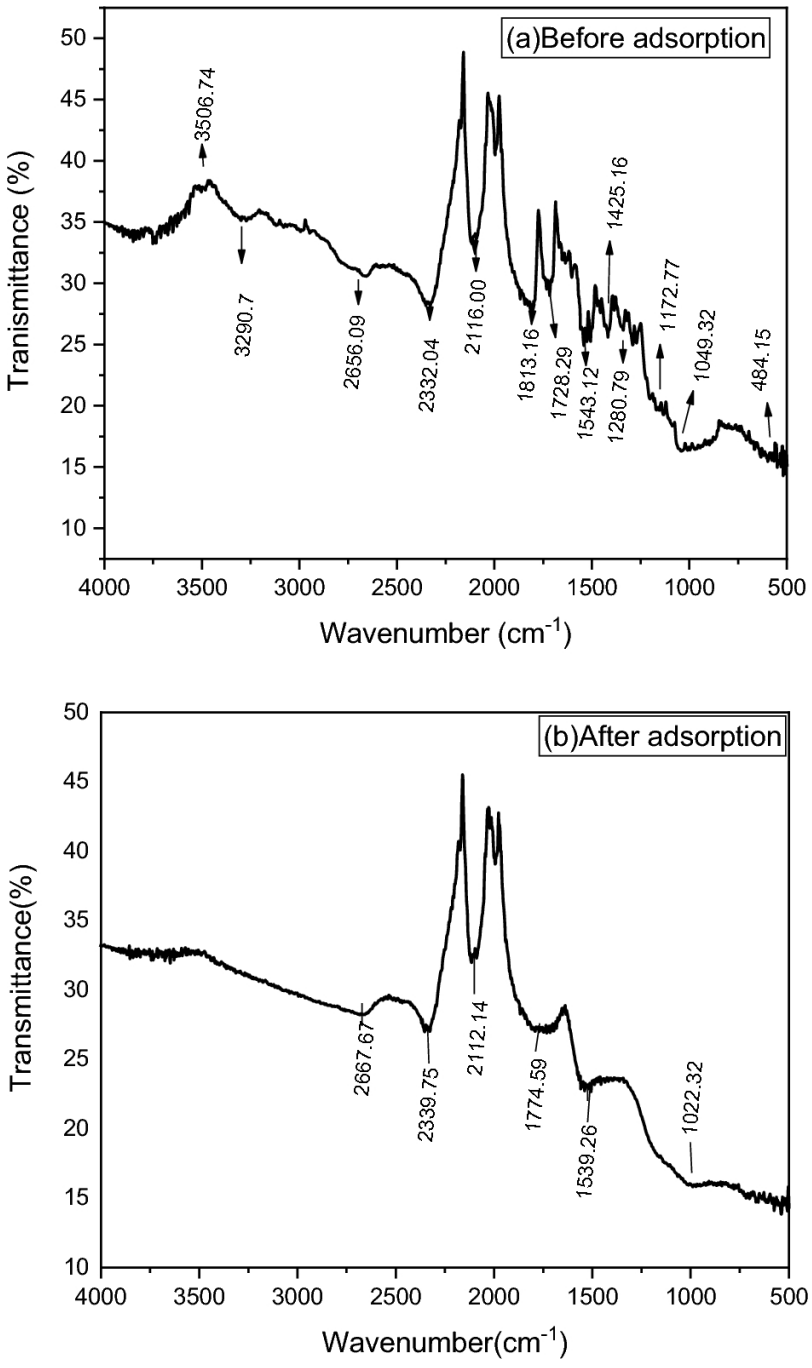


Figure 3. FTIR spectra of Rumex abyssinicus-derived activated carbon before (a) and after (b) adsorption of malachite green. Reproduced from Abewaa et al., Scientific Reports 2023, 13, 14701 (open access, CC BY) [6]. No original spectra were recorded for this review.

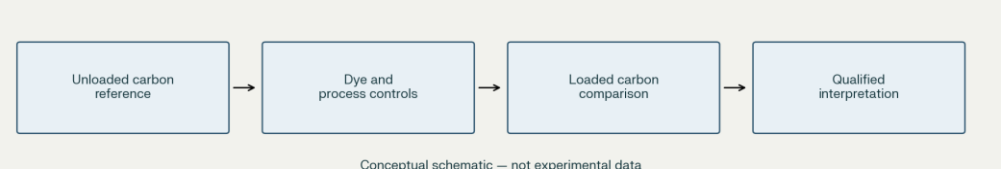


Figure 2. FTIR comparison strategy. No measured or simulated spectrum is shown.

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4. UV–Vis analysis and mass balance

Select the analytical wavelength from a spectrum recorded under the actual solution conditions. pH, aggregation and other absorbing species can alter the response. Within a validated linear range, the Beer–Lambert relation is:

$$A = \varepsilon l c \qquad (1)$$

A is dimensionless absorbance, ε is the molar absorption coefficient, l is optical path length and c is molar concentration, with consistent units. For mass-concentration calibration, A = aC + b gives C = (A − b)/a. Apply dilution corrections and do not impose a zero intercept without supporting calibration and blank results.

Validate separation of suspended carbon and assess losses to filters or vessels. Use dye-only controls to evaluate non-adsorptive changes and adsorbent blanks to detect leached absorbing species. Reduced absorbance at one wavelength does not by itself establish adsorption, degradation or mineralization. [9]

For a closed batch with constant volume and negligible alternative dye losses, uptake and apparent removal follow [3]:

$$q_e = (C_0 - C_e)V/m \qquad (2)$$

$$\text{Apparent removal (\%)} = 100(C_0 - C_e)/C_0 \qquad (3)$$

C_0 and C_e are initial and equilibrium concentrations (mg L^{-1}), V is liquid volume (L), m is dry adsorbent mass (g), and q_e is uptake (mg g^{-1}). Equation (3) requires $C_0 > 0$. Repeated sampling or liquid replacement requires accounting for volume changes and solute removed in aliquots. Assign solution depletion specifically to adsorption only after assessing relevant alternative losses. [9]

5. Equilibrium models

Establish equilibrium experimentally and report temperature, pH, concentration range and adsorbent dosage. The Langmuir expression is [3]: [11]

$$q_e = q_{max} K_L C_e / (1 + K_L C_e) \qquad (4)$$

q_{max} is the fitted limiting capacity (mg g^{-1}) and K_L is an affinity parameter (L mg^{-1}) for the units above. The idealized assumptions include equivalent sites, monolayer occupancy and no lateral adsorbate interactions. Agreement with the equation does not establish all these assumptions. A fitted q_{max} may be poorly constrained if saturation was not approached. [9,11]

The Langmuir model was originally developed for gas adsorption on idealized surfaces. Its application to aqueous dye adsorption is a modeling choice; a satisfactory fit should not be presented as direct confirmation that a heterogeneous activated-carbon surface satisfies every original assumption [9,11].
The Freundlich expression is [3]:

$$q_e = K_F C_e\text{^}(1/n) \qquad (5)$$

n is dimensionless and K_F has units (mg g^{-1})(L mg^{-1})^(1/n). This empirical expression may describe heterogeneous adsorption over a measured range, but it has no finite saturation limit and should not be extrapolated indefinitely.

Prefer nonlinear regression on the original measurement scale with an appropriate error model. Examine residuals, physical plausibility and parameter uncertainty. Linearization can change error structure; R^2 alone is insufficient for model selection or mechanism assignment. No fitted constants are reported because no numerical equilibrium dataset was supplied [3]. [9]

6. Kinetic models

Under the same closed-batch assumptions, $q_t = (C_0 - C_t)V/m$. For an initially unloaded adsorbent, commonly used empirical expressions are [4,5]:

Pseudo-first-order: $q_t = q_e\,[1 - \exp(-k_1\,t)]$ (6)

Pseudo-second-order: $q_t = k_2\,q_e^2\,t / (1 + k_2\,q_e\,t)$ (7)

For time in min and uptake in mg g^{-1}, k_1 is in min^{-1} and k_2 in g mg^{-1} min^{-1}. Compare fitted equilibrium uptake with independently determined values. Different initial conditions require an appropriate formulation.

The differential expression $dq_t/dt = k_2\,(q_e - q_t)^2$ does not by itself identify a microscopic reaction involving two sites or electron exchange. The transformed form $t/q_t = 1/(k_2\,q_e^2) + t/q_e$ is undefined at $q_t = 0$ and may yield misleadingly high transformed R^2 values. Fit original uptake or concentration data and inspect residuals [5].

A pseudo-second-order fit does not prove chemisorption or identify the rate-limiting step. External mass transfer, intraparticle transport and surface processes can all contribute to time dependence and require independent investigation [1,5]. [9]

7. Mechanistic interpretation and quality control

Assess electrostatic contributions using dye speciation and measured surface-charge behavior. Hydrogen bonding requires plausible donor–acceptor groups and supporting evidence. Aromatic FTIR bands alone do not prove π–π association. Pore-filling claims require pore-accessibility evidence in relation to the adsorbate. These mechanisms can coexist, but their relative importance cannot be established from this manuscript [1,2]. [9,12]

A critical review of aqueous adsorption studies identifies recurring problems in terminology, performance metrics, kinetic and equilibrium modeling, and mechanistic interpretation. The methodological safeguards used here are intended to avoid these problems, particularly the identification of a microscopic mechanism solely from a fitted kinetic equation or a spectral shift [9].

- Document complete preparation conditions, particle size, dry adsorbent mass and solution conditions.
- Report spectrometer settings, calibration, analytical range, blanks, dilution factors and processing procedures.
- Include relevant controls, independent replicates and a defined uncertainty measure.
- Supply raw spectra and numerical time-series and equilibrium data with units and sample identifiers.
- Report fitting methods, objective functions, residuals, parameter uncertainties and constraints. [9]
- Identify figures as conceptual, measured, simulated, reproduced or adapted, with sources and permissions as needed.

8. Conclusion

Spectroscopy and adsorption models provide complementary information, but defensible conclusions require analytical controls, reproducibility and evidence beyond isolated bands or fit statistics. Equilibrium and kinetic equations are descriptive tools rather than independent proofs of microscopic mechanism. Original experimental claims require traceable measurements, appropriate mass balances, uncertainty analysis and complementary characterization [1–12].

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