Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 91 (7–8) S238–S241 (2026) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Silica modified with choline chloride/urea DES for ligand-free Cu(II) adsorption

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J. Serb. Chem. Soc. 91 (7–8) (2026) 809–822

The equation for pseudo-first order (PFO) is described as follows:

$$\log(q_e - q_t) = \log q_e - \frac{k_1}{2.303} t \quad \text{(S-1)}$$

where k_1 is the rate constant of the pseudo-first-order model (min^{-1}), q_e is the amount of metal adsorbed at equilibrium (mg g^{-1}), and q_t is the amount of metal adsorbed at time t (mg g^{-1}). The value of k_1 and q_e was obtained from the plotted graph of $\log(q_e–q_t)$ against t.

Pseudo-second-order (PSO) equation by Ho and Mckay (1999) is as followed:

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t \quad \text{(S-2)}$$

where k_2 is the rate constant of pseudo-second order (g mg^{-1} min^{-1}). A graph of t/q_t *vs* t was plotted to find the initial adsorption rate, h (mg g^{-1} min^{-1}), and the half-equilibrium time, $t_{½}$ (min).

$$h = k_2 q_e^2 \quad \text{(S-3)}$$

$$t_{1/2} = \frac{k_2}{q_e} \quad \text{(S-4)}$$

The Langmuir isotherm describes the monolayer adsorption of an adsorbate onto the surface of an adsorbent containing a finite number of active sites. There will be no further sorption once an active site is filled up and the surface reaches a saturation point where the maximum adsorption is achieved.

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The isotherm is represented as:

$$\frac{C_e}{q_e} = \frac{1}{q_m} C_e + \frac{1}{bq_m} \quad \text{(S-5)}$$

where C_e is the equilibrium concentration of the adsorbate (mg L^{-1}), q_m is the adsorption capacity (mg g^{-1}), and b is the rate of adsorption (L mg^{-1}). The features of the parameter for Langmuir adsorption isotherm can be used to predict the affinity between the adsorbate and adsorbent using a dimensionless constant called the separation factor or equilibrium parameter (R_L), which is expressed by the following relationship:

$$R_L = \frac{1}{1 + bC_0} \quad \text{(S-6)}$$

Where C_0 is the initial adsorbate concentration (mg L^{-1}), R_L stipulates the favourability of the adsorption nature, either irreversible (R_L = 0), favorable ($0<R_L<1$), linear (R_L = 1) or unfavorable (R_L > 1). The values of linear regression coefficient (R^2) is 0.9887, demonstrating that the experimental data fitted well with the Langmuir isotherm equation. The R_L value in the present investigation was found to be 0.0911, indicating that the adsorption of the Cu (II) ions onto DES-Si is favorable, with the maximum adsorption capacity (q_m) of 17.54 mg g^{-1}.

The Freundlich isotherm describes the heterogeneous adsorption between adsorbate and adsorbent with a non-uniform distribution of heat of adsorption. The Freundlich isotherm is represented by the following Equation:

$$\log q_e = \log K_F + \frac{1}{n} \log C_e \quad \text{(S-7)}$$

Adsorption capacity, K_F, (mg g^{-1}) and Freundlich exponent, n can be found by plotting graph of log q_e versus log C_e. The n value indicated the type of sorption process to be chemical process if n <1 and physical process if n >1. As shown in Table V, it can be found that the value of R^2 is 0.976. In the present study, since n value is larger than 1, it indicates the physical adsorption of Cu (II) ions onto DES-Si.

The Temkin isotherm is a model that assumes the heat of adsorption (function of temperature) of the adsorbate in the layer would decrease linearly with the surface coverage due to adsorbent–adsorbate interactions. The equation of Temkin model is written as:

$$q_e = \frac{RT}{b_T} \ln S_T + \frac{RT}{b_T} \ln C_e \quad \text{(S-8)}$$

Where b_T (J mol^{-1}) is the Temkin constant related to the heat of adsorption and S_T (L g^{-1}) is the Temkin isotherm equilibrium binding constant. As shown in Table V, it can be found that the value of R^2 is 0.9914, suggesting that these

experimental data fit very well with the Temkin isotherm model. The following values were estimated: S_T = 6.4887 L g^{-1}, b_T = 711.17 J mol^{-1}, which are indications of the heat of sorption and physical adsorption process, respectively.

Dubinin-Radushkevich isotherm is a model that is commonly used to describe the mechanism of adsorption onto a heterogeneous surface and can be applied to determine the mean of adsorption energy (E) of the adsorbate. This adsorption energy is used to remove the adsorbate from the sorption space using the equation below:

$$E = \frac{1}{\sqrt{2\beta}} \tag{S-9}$$

where β is the DR model constant (mol^2kJ^{-1}). The value of E is important as it can be used to determine the type of adsorption of metal ions, either physical or chemical adsorption. The linear equation of this model is represented as:

$$\ln q_e = \ln q_m - \beta E^2 \tag{S-10}$$

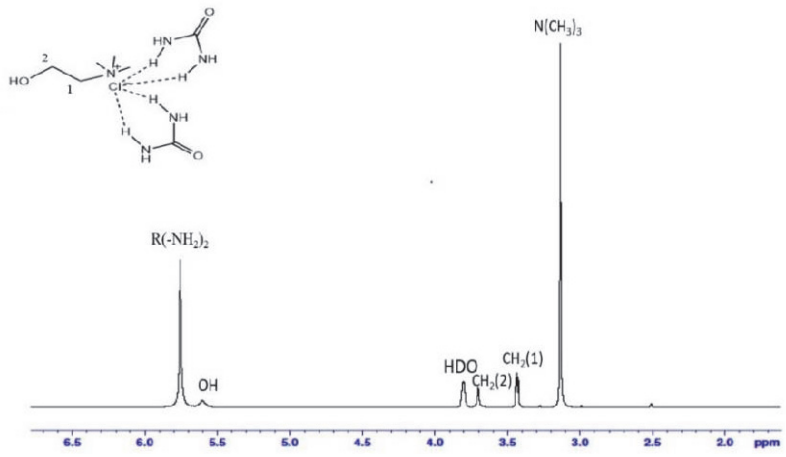

Fig. S1(a) ^{1}H-NMR spectrum of DES

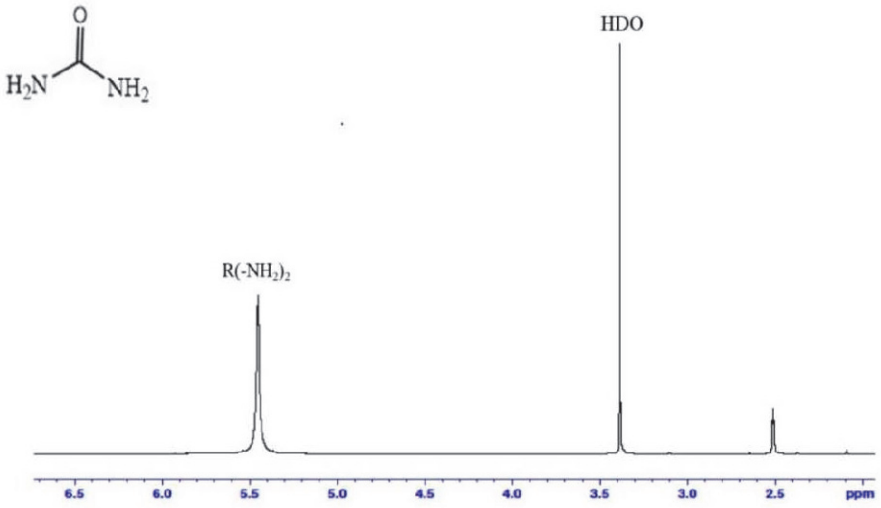

Fig. S1(b) ^{1}H-NMR spectrum of urea

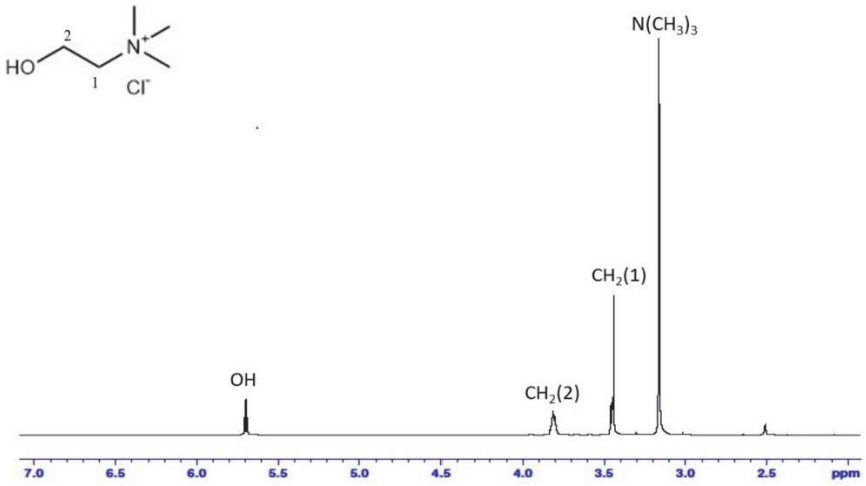

Fig. S1(c) ^{1}H-NMR spectrum of choline chloride.