List of Supplementary Materials

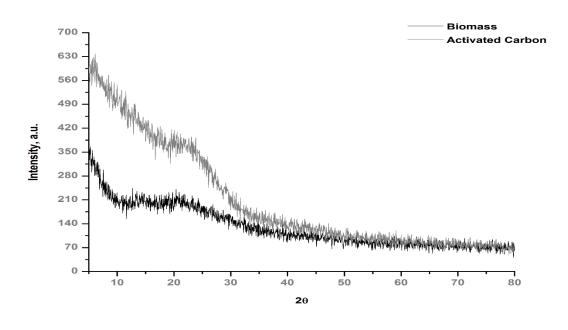
2 Powder X-ray Diffraction Analysis

3 Raw material (*Reptonia Buxifollia* seeds) and ACs prepared from raw material were investigated

4 using XRD which is illustrated in Fig. 1. The figure indicates AC exhibit broad diffraction peaks

- 5 at two theta position of 25° which, clues for presence of graphitic carbon. However, the absence of
- 6 sharp diffraction peak at 2Θ of 25° reveals a predominantly amorphous structure, which is an

7 advantageous property for well-defined porous materials[1].



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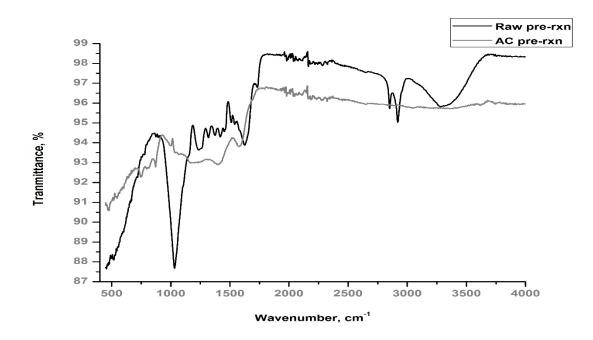
9 Fig. 1. X-ray Diffraction of R.B seeds and ACs

10 Fourier Transform Infrared (FTIR) Analysis

The chemical composition of raw (*Reptonia Buxifolia* seeds) and ACs prepared from raw material 11 were determined by Fourier Transform Infrared (FTIR) as shown in Fig. 2. The result of raw 12 material shows a presence of the various functional groups which include hydroxyl groups, amines, 13 various unsaturated hydrocarbons, aldehydes and carbonyl compounds. However, pyrolysis causes 14 loss of some of these peaks in ACs. In raw sample the broad band was observed at 3285 cm⁻¹. This 15 band is matched to stretching vibration of hydroxyl group on the surface. The sharp band observed 16 at 2919 cm⁻¹ and 2850 cm⁻¹ are due to the asymmetric and symmetric stretching of the methylene 17 18 C-H bond respectively. However, these peaks disappeared in ACs, as ACs loss these functional

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19 groups in heat treatment. The band observed at 2162 cm⁻¹(Fig. 3) corresponds to presence of 20 silane(Si-H) groups [2]. The band due to silane was also retained in ACs. The band observed at 21 1235 cm⁻¹ is matching to stretching vibration of C-O. The band found at 1627 cm⁻¹ and 1032 cm⁻¹ 22 were due to the presence of phenol. In ACs new peaks at 1404 cm⁻¹ is observed which might be 23 due to the carbonate group develop in ACs.



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25 Fig. 2. FTIR spectra of raw material and ACs

26 **Pseudo-1**st Order Kinetic Equation

A pseudo-1st-order kinetic model successfully explains the kinetics of many adsorption systems.
The Lagergren equation is given as follows[3].

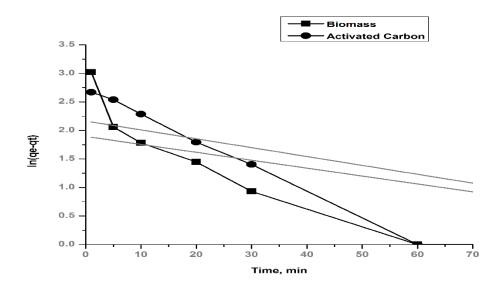
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$$\ln(q_e - q_t) = \ln q_e - k_1 t \tag{1}$$

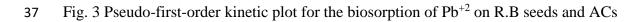
Where, q_t is the amount of Pb⁺² adsorbed (mg/g) at any time t, q_e is the amount of Pb⁺² adsorbed (mg/g) at equilibrium, and k_1 is the rate constant.

The value of k_1 can be evaluated from the intercept and slope of the linear plot of $ln(q_e-q_t)$ against time t as shown in Fig. 2. From the plot the value of correlation coefficient R^2 was found to be 0.687 and 0.824 for biomass and activated carbon, respectively. The value of R² obtained suggests

that the adsorption of Pb^{+2} ions on biomass does not follow the pseudo-first-order kinetics.



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38 Thermodynamics of Pb⁺² Adsorption

The nature of the adsorption of Pb^{+2} on the biomass and ACs was estimated by varying different thermodynamic parameters such as free energy (ΔG^0) and K₀ by the following equation [4].

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$$\Delta G^0 = -RT ln K_0 \tag{2}$$

42 Where K_0 is the equilibrium constant and determined as:

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$$K_0 = \frac{a_s}{a_e} = \frac{v_s}{v_e} \frac{c_s}{c_e}$$
 (3)

44 Where, C_s represents Pb^{2+} amount adsorbed per mass of Adsorbent (mol/g) and C_e shows the Pb^{2+} 45 concentration in solution at equilibrium (mol/ml), a_s is the activity of adsorbed Pb^{2+} , a_e is the 46 activity of the Pb^{2+} in solution at equilibrium, v_s is the activity coefficient of the adsorbed Pb^{2+} and 47 v_e is the activity coefficient of the Pb^{+2} in solution. The K₀ values were used to determine ΔG^0 , 48 ΔH^0 and ΔS^0 . 49 The average standard enthalpy change (ΔH°) of the system was calculated by using Van't Hoff 50 equation:

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$$lnK_0(T_2) - lnK_0(T_1) = \frac{-\Delta H^0}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$
(4)

52 Where, T_2 represent final temperature and T_1 represent initial temperature. The standard entropy 53 change (ΔS^0) can be obtained by the equation:

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$$\Delta S^0 = \frac{\Delta G^0 - \Delta H^0}{T}$$
(5)

The Thermodynamic parameters of biomass and activated carbon are listed below in Table I and Table II, respectively. A negative value of enthalpy change clues that Pb⁺² adsorption on biosorbent is exothermic process, which is supported by the decreasing adsorption of Pb⁺² when temperature was increased from 283K to 343K. A negative standard free energy change shows that the adsorption reaction is a spontaneous and reversible process.

60 TABLE I. Thermodynamic parameters values for Lead ion adsorption on raw biomass

Thermodynamic	Temperature (K)								
constants	283	293	303	313	323	333	343		
$K_o(mLg^{-1})$	1118.12	713.59	295.93	245.60	176.77	149.01	51.51		
$\Delta G^{o}(\text{kcal}_{\text{th}} \text{ mol}^{-1})$	-3.95	-3.83	-3.43	-3.42	-3.32	-3.31	-2.69		
$\Delta H^{o}(kcal_{th} mol^{-1})$	-8.87	-8.87	-8.87	-8.87	-8.87	-8.87	-8.87		
$\Delta S^{o}(kcal_{th} mol^{-1})$	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02		

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Thermodynamic constants	Temperature (K)								
	283	293	303	313	323	333	343		
$K_o(mLg^{-1})$	1459.25	1091.34 3	1061.72	955.69	902.60	769.29	600.35		
$\Delta G^{o}(kcal_{th} mol^{-1})$	-4.097	-4.07	-4.195	-4.27	-4.37	-4.397	-4.36		
$\Delta H^{o}(kcal_{th} mol^{-1})$	-2.42	-2.42	-2.42	-2.42	-2.42	-2.42	-2.42		
$\Delta S^{o}(kcal_{th} mol^{-1} deg^{-1})$	0.006	0.006	0.006	0.006	0.006	0.006	0.006		

68 TABLE II. Various thermodynamic parameters values for Lead ion adsorption on ACs

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72 Reference

73 [1] M.S. Shamsuddin, N.R.N. Yusoff, M.A. Sulaiman, Procedia Chemistry 19 (2016) 558.

74 [2] D.B. Kapgate, C. Das, D. Basu, A. Das, G. Heinrich, Rubber composites based on silane-

treated stöber silica and nitrile rubber: Interaction of treated silica with rubber matrix, 2013.

76 [3] Z.A. Jamiu, T.A. Saleh, S.A. Ali, RSC Advances **5** (2015) 42222.

[4] Ç. Arpa, E. Başyilmaz, S. Bektaş, Ö. Genç, Y. Yürüm, Fuel Processing Technology 68
(2000) 111.

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