Electronic Supplementary Material (ESI) for Dalton Transactions.

Evaluation of bishexadecyltrimethyl ammonium palladium tetrachloride based dual functional colloidal carrier as an antimicrobial and anticancer agent

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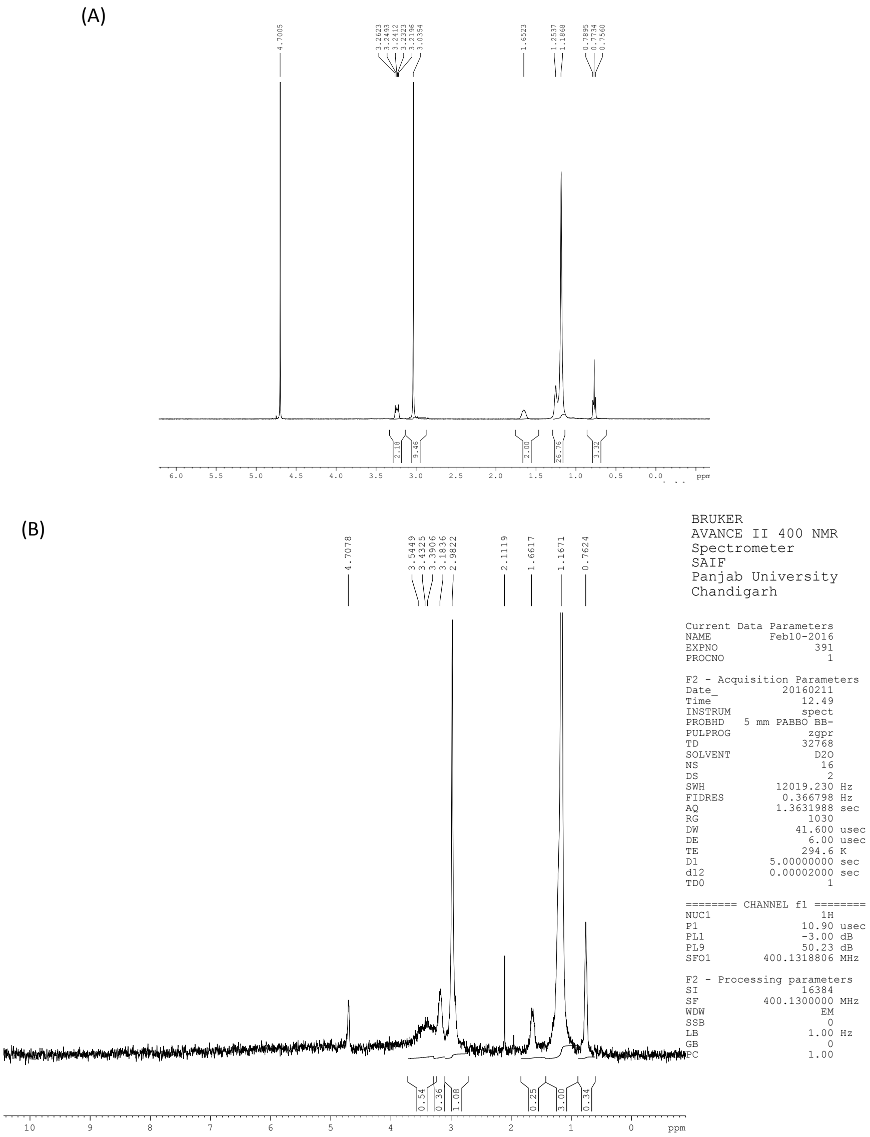

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Spectrometer
SAIF
Panjab University
Chandigarh

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Figure ES1. NMR spectra of (A) CTAC, (B) PdCTAC.

Thermogravimetric analysis

For solid state reaction, rate constant (k) is calculated by kinetic eqn.

$$\frac{d\alpha}{dt} = kf(\alpha) = Ae^{-\frac{E}{RT}}f(\alpha) \qquad (1)$$

where, A (pre-exponential factor) and E (activation energy) are the Arrhenius parameters; α is the fractional reaction; t is time; R is the gas constant; T is temperature in Kelvin, and f (α) is the kinetic function.

In isothermal kinetic studies, the rate constant is given by:

$$g(\alpha) = kt \qquad (2)$$

where, $g(\alpha) = \int_0^\infty \frac{d\alpha}{f(\alpha)}$ can be calculated by the integration of f(α).

Under non-isothermal conditions, in which a sample is heated at a constant rate β=d*T/*dt, the explicit temporal in equation (3) is eliminated through the trivial transformation, so that $T=T_0+\beta$, where T_0 is the starting temperature and T is the temperature at any time *t.* Upon integration, eq. (1) may be written as:

$$g(\alpha) = \frac{A}{\beta}\int_{T_O}^{T} e^{-E/RT}dt \qquad (3)$$

Doyle's equation leads by Integration of equation (3) by considering that reaction rate is negligible at low temperatures

$$g(\alpha) = \frac{AE}{R\beta}\int_{T_O}^{T}\frac{e^{-x}}{x} - \int_{0}^{\infty}\frac{e^{-u}}{u}du = \frac{AE}{R\beta}P(x) \qquad (4)$$

where, *u=E/RT* and *x* is the corresponding value of *u* at which a fraction of material has been decomposed. The above equation can be reformulated as:

$$\ln g(\alpha) - \ln P(x) = \frac{AE}{R\beta} = B \tag{5}$$

where, B is a constant for a particular reaction at a constant heating rate. The integral function P(x) has no analytical solution; it may be written in an expanded form and estimated by using a procedure of trial-and-error type involving iteration.

(i) *Coats-Redfern method*

$$g(\alpha) = \frac{ART^2}{\beta E}\left[1 - \frac{2RT}{E}\right] e^{-E/RT} \tag{6}$$

So the equation takes the form:

$$-\ln\frac{g(\alpha)}{T^2} = -\ln\frac{AR}{\beta E}\left[1 - \frac{2RT}{E}\right] + \frac{E}{RT} \tag{7}$$

The fraction mass loss (α) and corresponding $(1–\alpha)^n$ are calculated from TG curves, where *n* depends upon the reaction model.

$$-\log\frac{1-(1-\alpha)^{1-n}}{T^2(1-n)} = \log\frac{AR}{\beta E}\left[1 - \frac{2RT}{E}\right] - \frac{E}{2.303RT} \qquad \text{for } n \neq 1 \tag{8}$$

$$-\log\frac{-\log(1-\alpha)}{T^2} = \log\frac{AR}{\beta E}\left[1 - \frac{2RT}{E}\right] - \frac{E}{2.303RT} \qquad \text{for } n=1 \tag{9}$$

In general, $2RT/E<<1$ exhibits a small variation with T. So, it is assumed that the term (1–2RT/E) is approximately constant and equal to unity. Therefore, plotting the left hand side of the above equations against $1/T$ gives the slope $-2.303E/R$ which yields the value of activation energy and the intercept gives value of *A* with excellent correlation coefficients, which indicates a good fit of the linear function.

(ii) *Madhusudanan- Krishnan-Ninan method*

$$-\ln\frac{g(\alpha)}{T^{1.9206}} = -\ln\frac{AR}{\beta E} + 3.7678 - 1.9206\ln E - 0.12040\frac{E}{RT} \tag{10}$$

(iii) *Wanjun–Yuwen–Hen–Cunxin method*

$$-\ln\frac{g(\alpha)}{T^{1.8946}} = -\ln\frac{AR}{\beta E} + 3.6350 - 1.8946\ln E - 1.0014\frac{E}{RT} \tag{11}$$

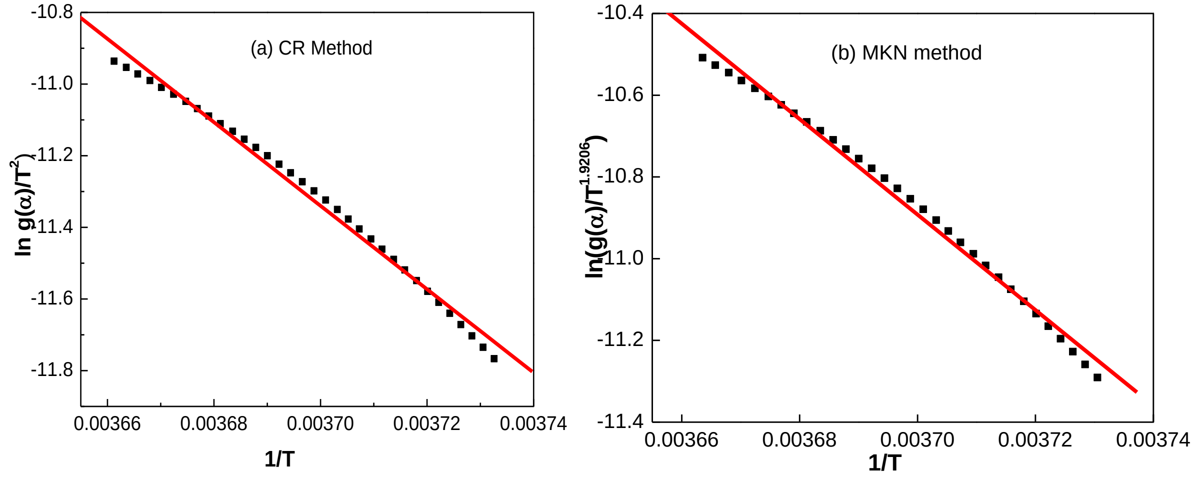
(iv) *Van Krevelen method*

$$\ln g(\alpha) = \ln\left(\frac{A(0.368/T_m)^{\frac{E_a}{RT_m}}}{\beta(\frac{E_a}{RT_m}+1)}\right) + \left(\frac{E_a}{RT_m}+1\right)\ln T \tag{12}$$

(v) *Horowitz–Metzger method*, a new parameter T = $T_m + \theta$ has been introduced. If the order of reaction is 1, T_m is defined as the temperature at which $(1 - \alpha)_m = 1/e = 0.368$ and the final expression is:

$$\ln\ln(\alpha) = \frac{E\theta}{RT_m^2} \tag{13}$$

In the above equations; α, g(α), β, T_m, *E, A, R* are the degree of reaction, integral function of conversion, heating rate, DTG peak temperature, activation energy (kJ mol^{-1}), pre-exponential factor (min^{-1}) and gas constant (8.314 $\text{Jmol}^{-1}\text{K}^{-1}$), respectively.



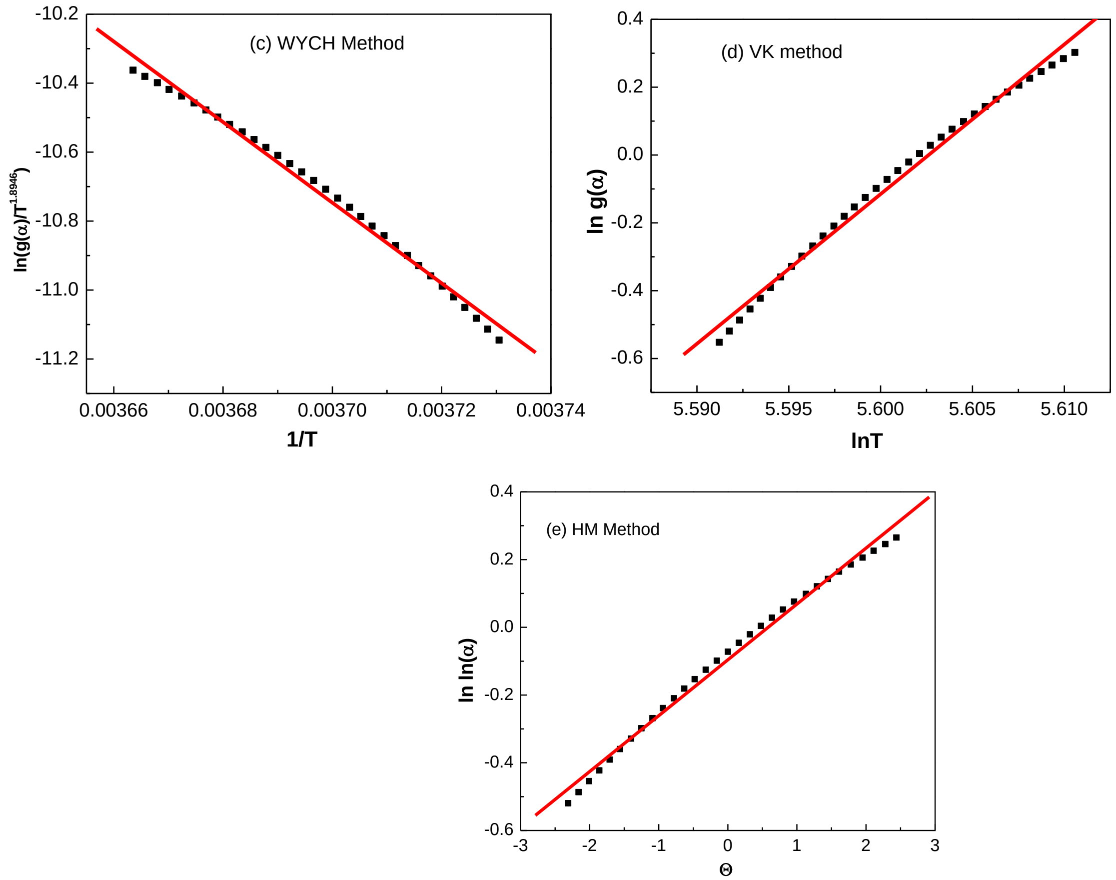


Figure ES2: Linearization curves obtained by (a) Coats–Redfern (CR), (b) Madhusudanan–Krishnan–Ninan (MKN), (c) Wanjun–Yuwen–Hen–Cunxin (WYHC), (d) van Krevelen (vK) methods and (e) Horowitz–Metzger (HM) methods for PdCTAC.

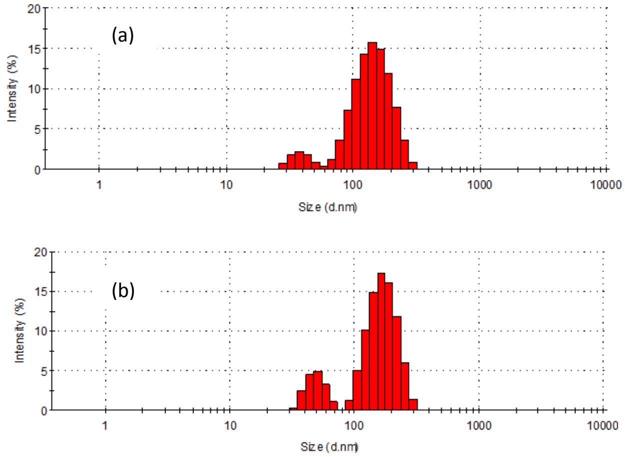


Figure ES3: the hydrodynamic radius of (a) freshly prepared metallomicelles (b) after one week

Table S1: Stern Volmer constant, binding constant and number of binding sites of BSA with premiceller system of Pd:CTAC

K_{SV} (10^3 $Lmol^{-1}$)	15.84
K_a (10^3 $Lmol^{-1}$)	17.74
n	1.3
R	0.997

Table S2: Colony formation at various dilutions against different microbes

Microbes		Colony formation at various dilutions of 0.5 mg/ml				
	Dilutions →	$0.5X10^{-1}$	$0.5X10^{-2}$	$0.5X10^{-3}$	$0.5X10^{-4}$	$0.5X10^{-5}$
E.coli	CTAC	N	C	C	C	C
	PdCTAC	60	130	C	C	C
S.aureus	CTAC	35	C	C	C	C
	PdCTAC	40	80	C	C	C
A. niger	CTAC	0	55	C	C	C
	PdCTAC	1	60	116	128	240
A. fumigatus	CTAC	0	0	C	C	C
	PdCTAC	3	7	12	24	C
C.lunata	CTAC	N	N	C	C	C
	PdCTAC	88	148	200	248	432
H.oryzae	CTAC	N	N	12	C	C
	PdCTAC	32	36	78	128	192

‘confluent’, represented by ‘C’, where the growth of colonies was vigorous that no margins were observed

“non confluent’ is represented by ‘N’ where no growth of colonies was observed