Effect of Physical Chemical Parameters on photocatalysis of TiO_2 anatase

Effet des Paramètres Physico-chimiques améliorant la photocatalyse de TiO_2 anatase

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Modelling of the photocatalytic tests

The experimental evolution of MB degradation as a function of time was fitted with a 3rd degree polynomial:

$(a_0 + a_1.x + a_2.x^2 + a_3.x^3)$ (1)

The variation of all coefficients (a_0 to a_3) was further fitted in order to provide a complete 3D map evaluation of the MB degradation as a function of time and other variables.

For each experimental curve, coefficients a_0 to a_3 were determined by a least square fit, and these values were used for interpolation between the experimental points. A response surface map was then calculated by using the fit equation of each coefficient.

Table S1: Reliability Coefficients R^2 of the linear fits for the modelling of a zero-order (Ct=f(t)), first order (Ln(Ct)=f(t)), and second order (1/Ct=f(t)) kinetics (Graphs in Figures S9). Fits were done within The 40-200 min time range was selected as the fitting range to avoid initial and final conditions.

TiO_2 (mg)	zero order	first order	second order
5	**0.986**	*0.968*	*0.963*
10	**0.967**	*0.945*	*0.917*
20	**0.966**	*0.920*	*0.867*
50	**0.989**	*0.974*	*0.959*
100	**0.872**	*0.828*	*0.777*
200	*0.981*	**0.982**	**0.982**
300	**0.9338**	*0.904*	*0.869*

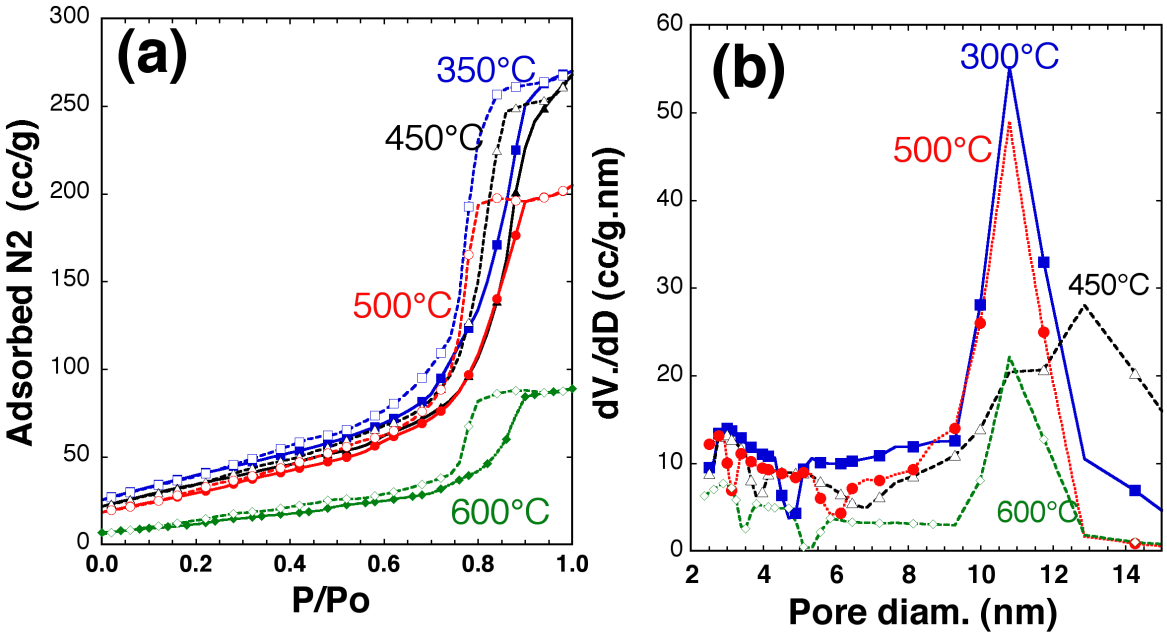


Figure S1: N_2 isotherm adsorption (a) and pore size distribution (b) for the TiO_2 anatase thermally treated at different temperatures.

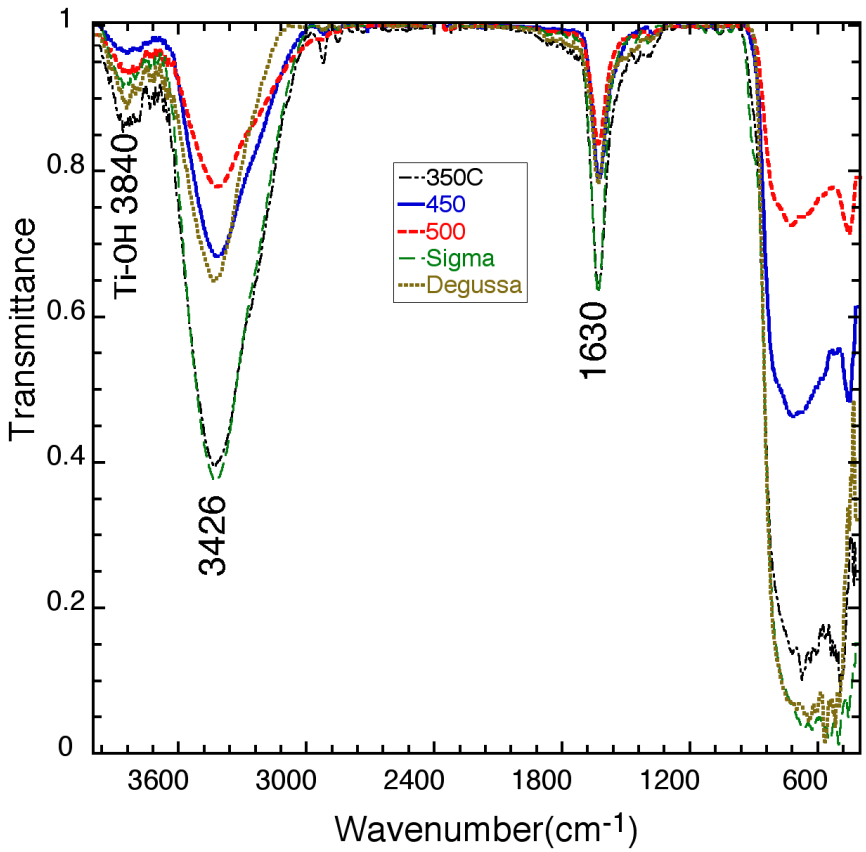


Figure S2: FT-IR spectra of T350, T450, T500, and Sigma and Degussa commercial TiO_2 powders

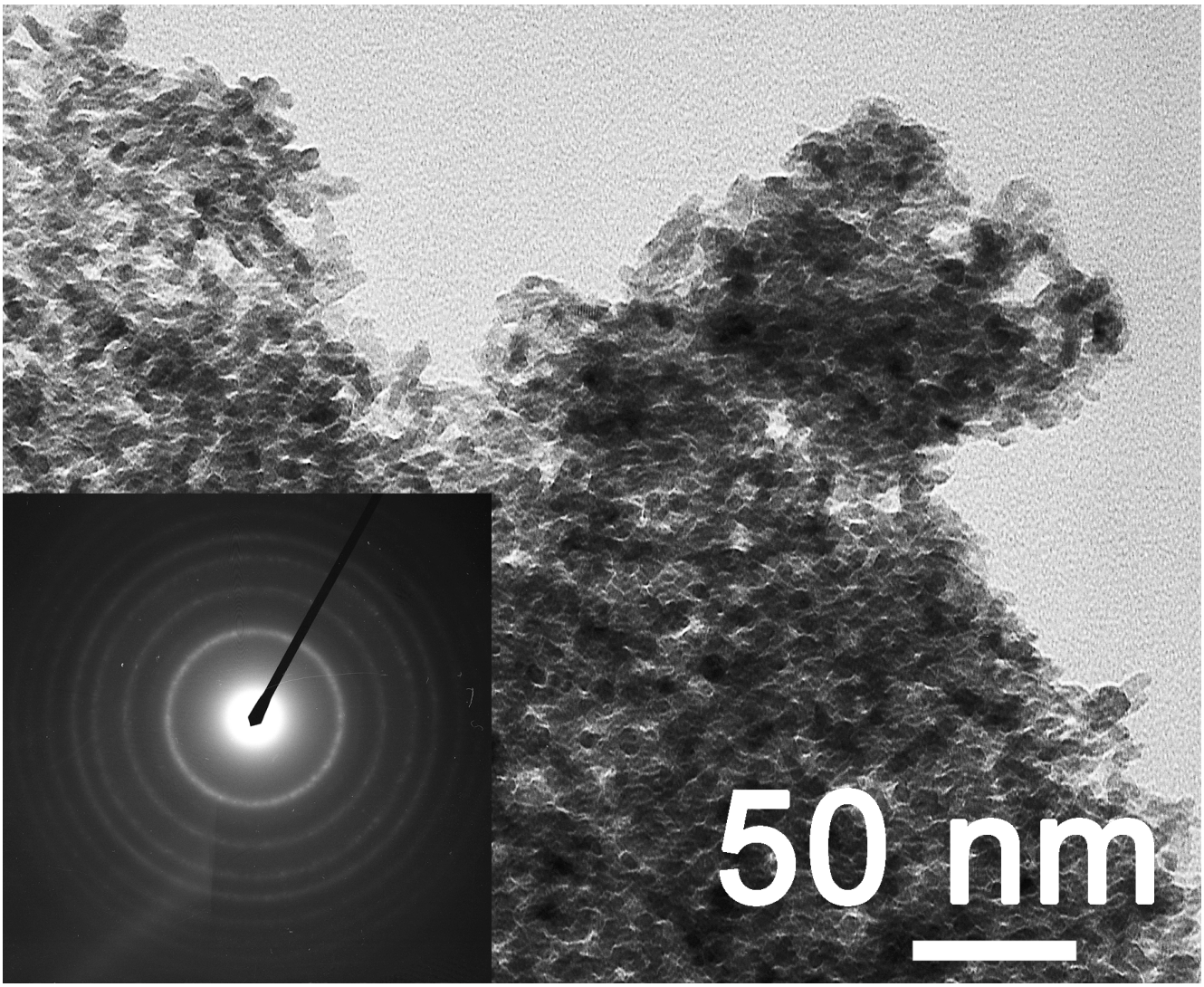


Figure S3: TEM micrography of RT-TiO_2

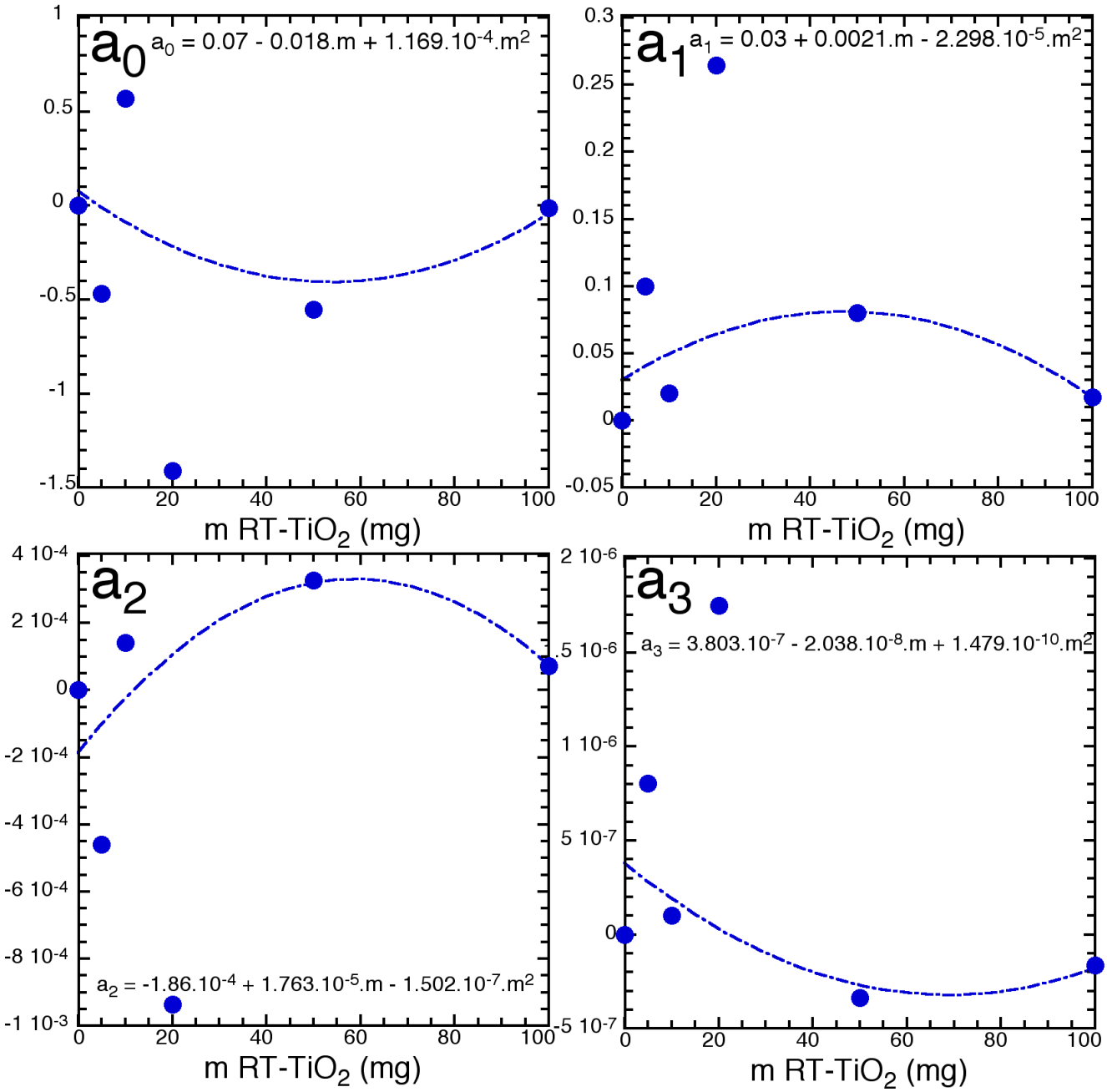


Figure S4: Values (dots) and 2nd order fit (dashed lines) of the polynomial parameters $a_0(m)$ to $a_3(m)$, with m the mass of RT-TiO_2, and the parameters $a_0(m)$ to $a_3(m)$ being the variable of the 3rd order degree polynomial [%(degrad) = $a_0(m) + a_1(m).t + a_2(m).t^2 + a_3(m).t^3$]. Due to large discrepancy, the values of the 20 mg samples were not used for fitting.

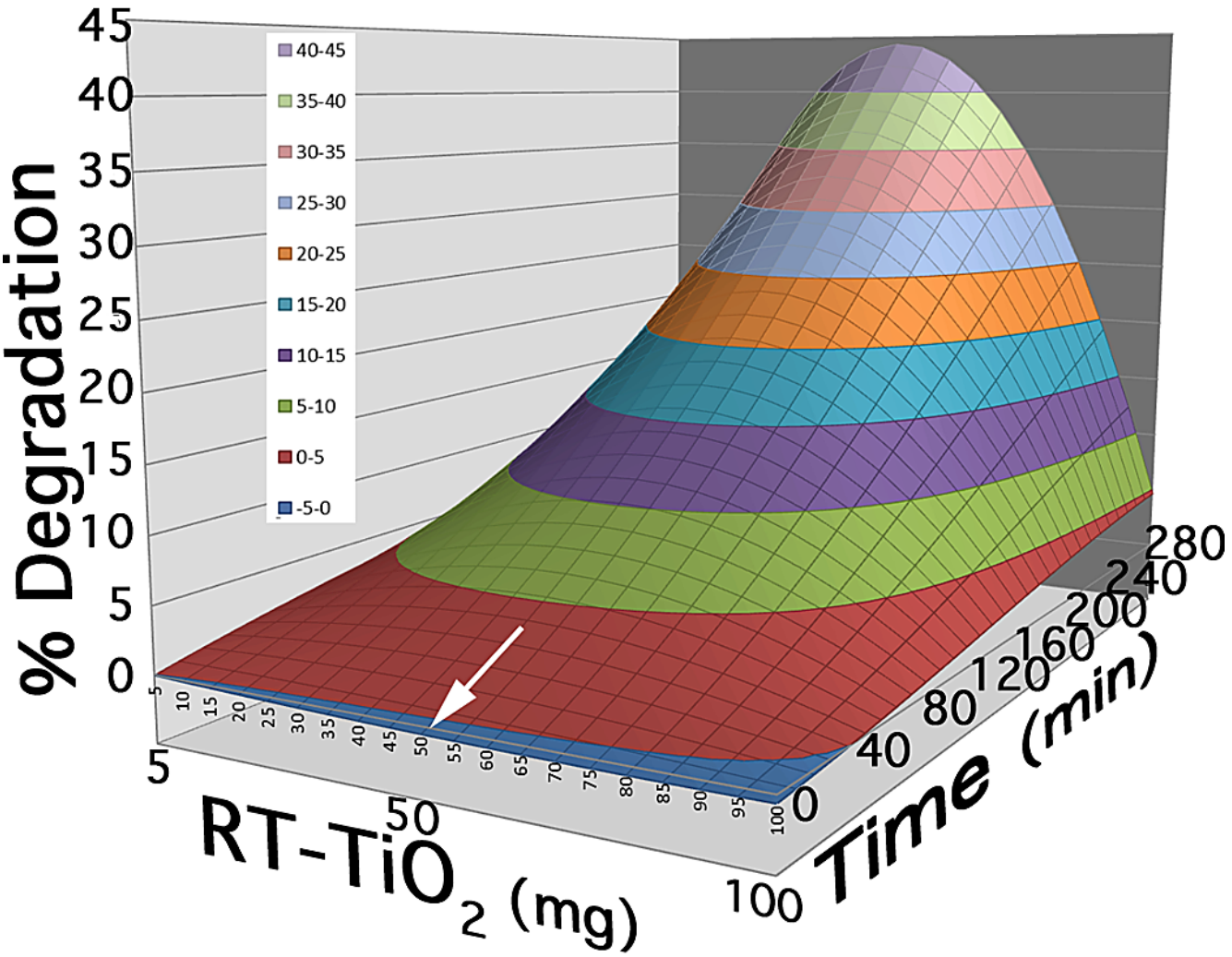


Figure S5: Modelling of the MB Degradation as a function of time (0 to 280 min) and mass of catalyst (5 to 100 mg), for RT-TiO_2.

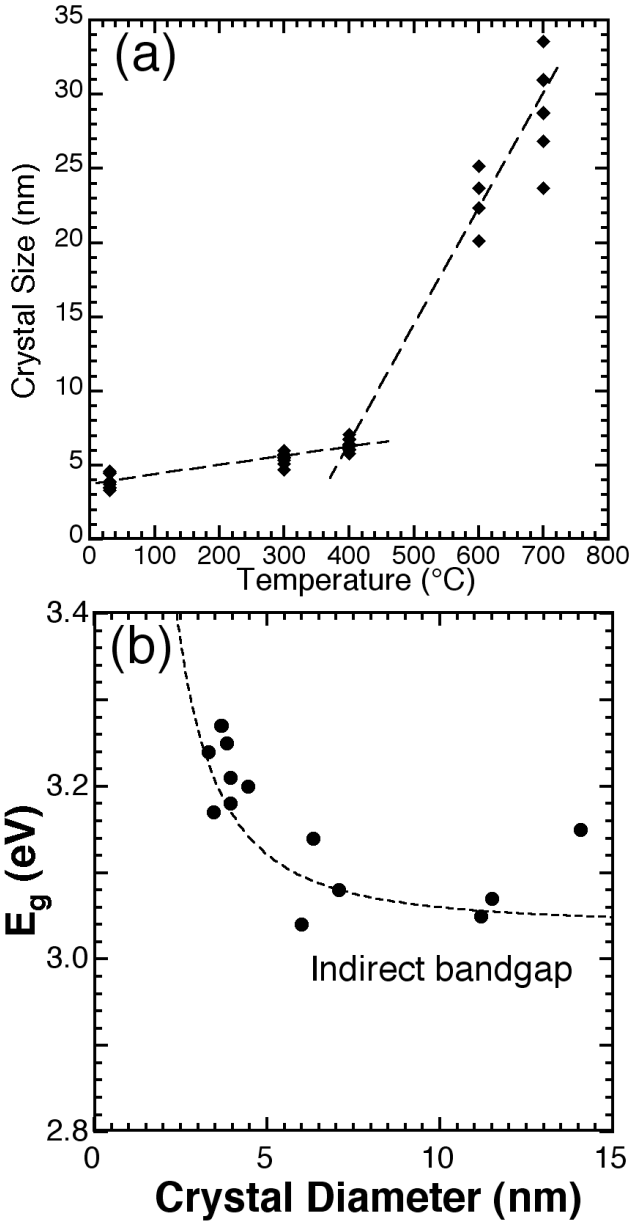


Figure S6: (a) Evolution of the crystal size of RT-TiO_2 as a function of the temperature, and (b) correlation between the measured band gap (indirect band gap model) and the crystal size.

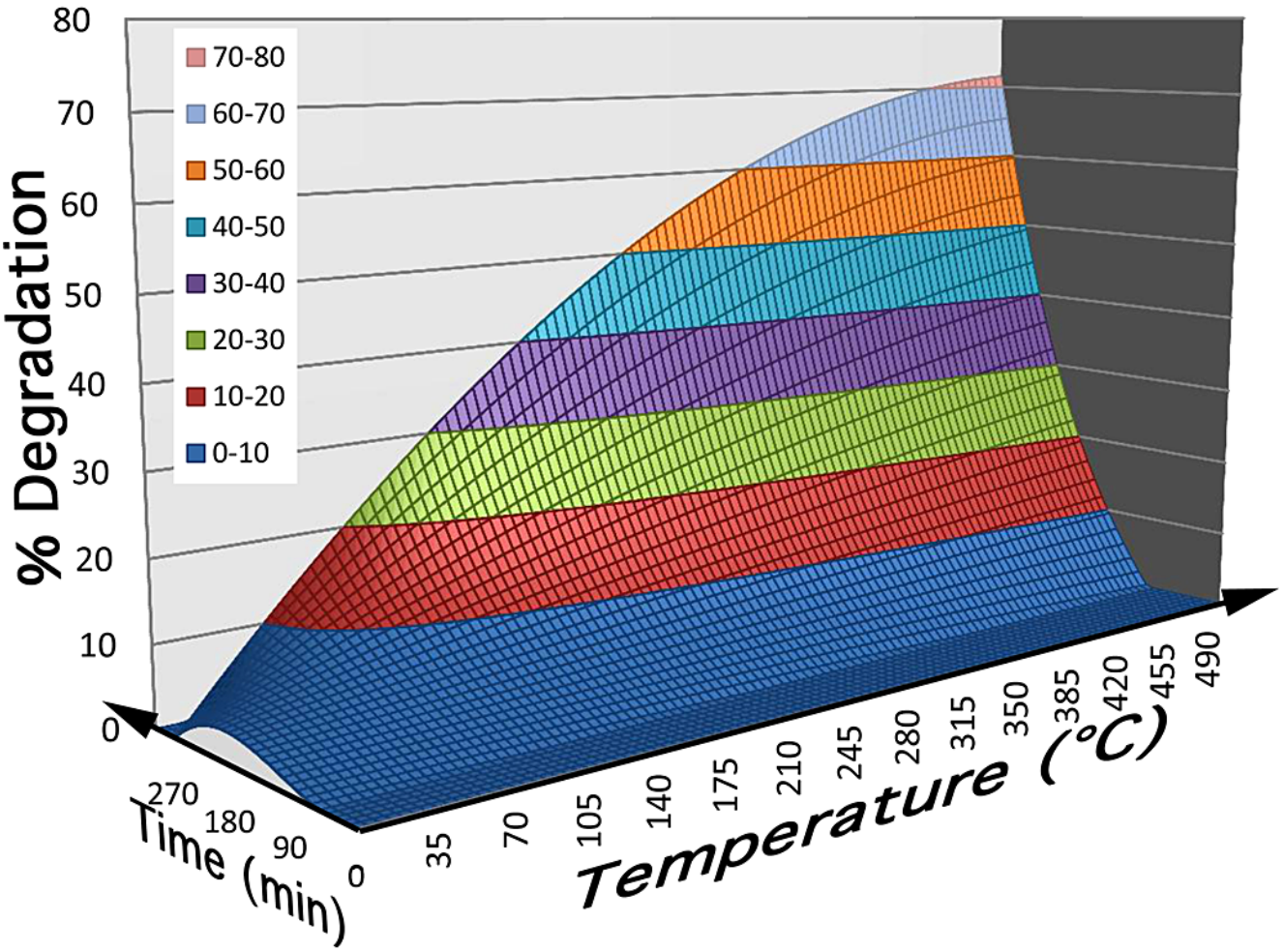


Figure S7: Modelling of the MB Degradation as a function of time (0 to 300 min) and temperature of catalyst activation (0 to 500°C), for an initial 100 mg RT-TiO_2 sample.

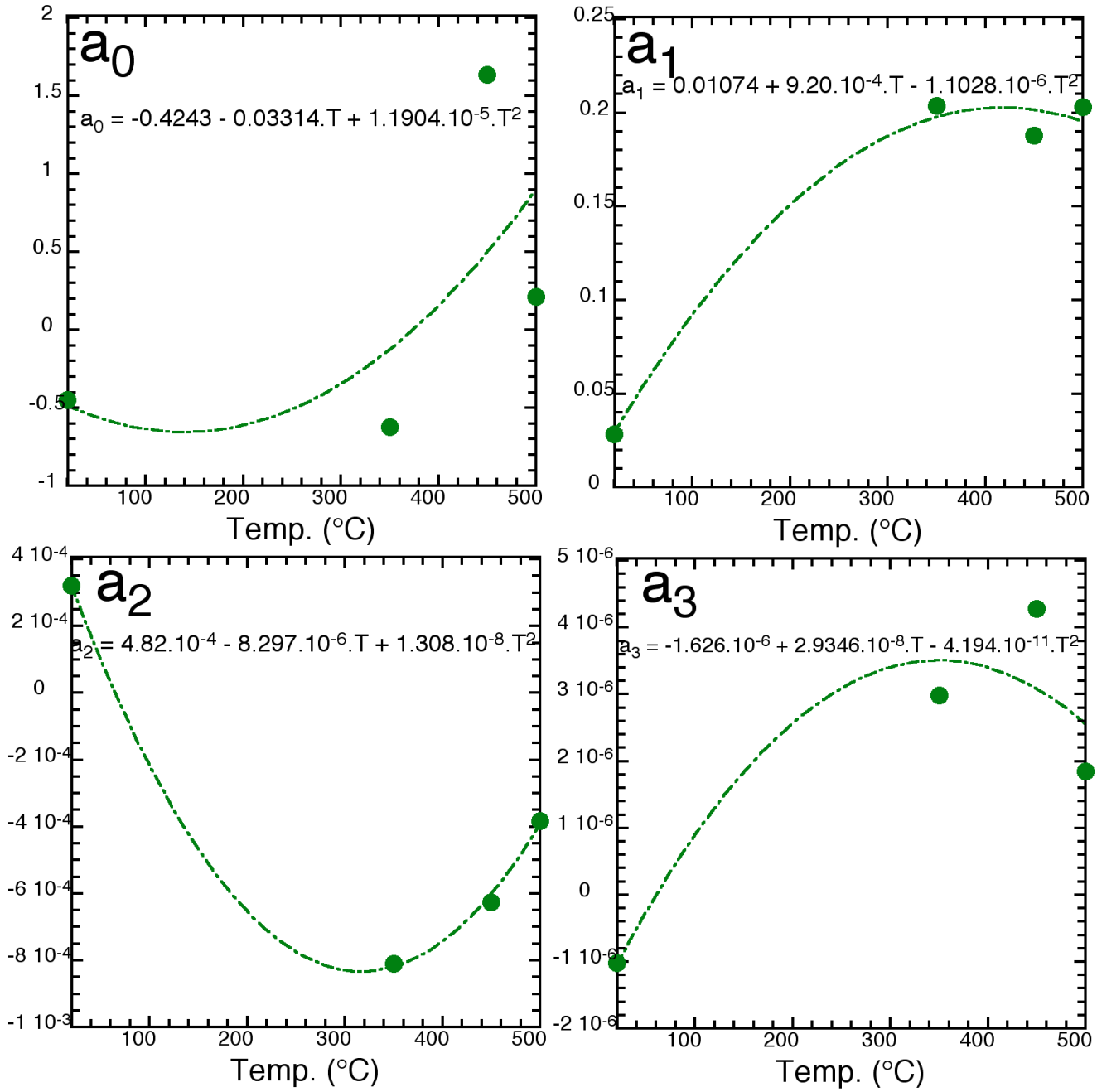


Figure S8: Values (dots) and 2nd order fit (dashed lines) of the polynomial parameters $a_0(T)$ to $a_3(T)$, for 100 mg of RT-TiO_2, activated at different temperatures. $a_0(T)$ to $a_3(T)$ being the variable of the 3rd order degree polynomial [%(degrad) = $a_0(T) + a_1(T).t + a_2(T).t^2 + a_3(T).t^3$].

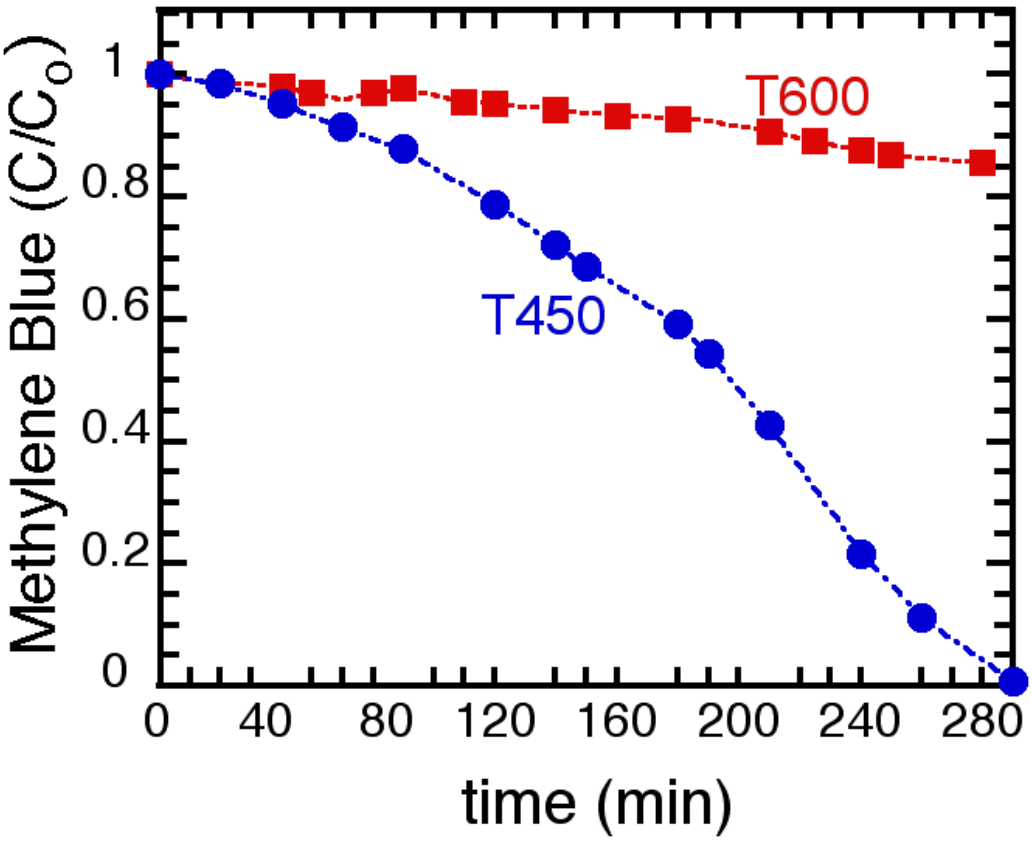


Figure S9: Comparison in the photodegradation of Methylene Blue between a 20 mg sample activated at 450°C and 600°C.

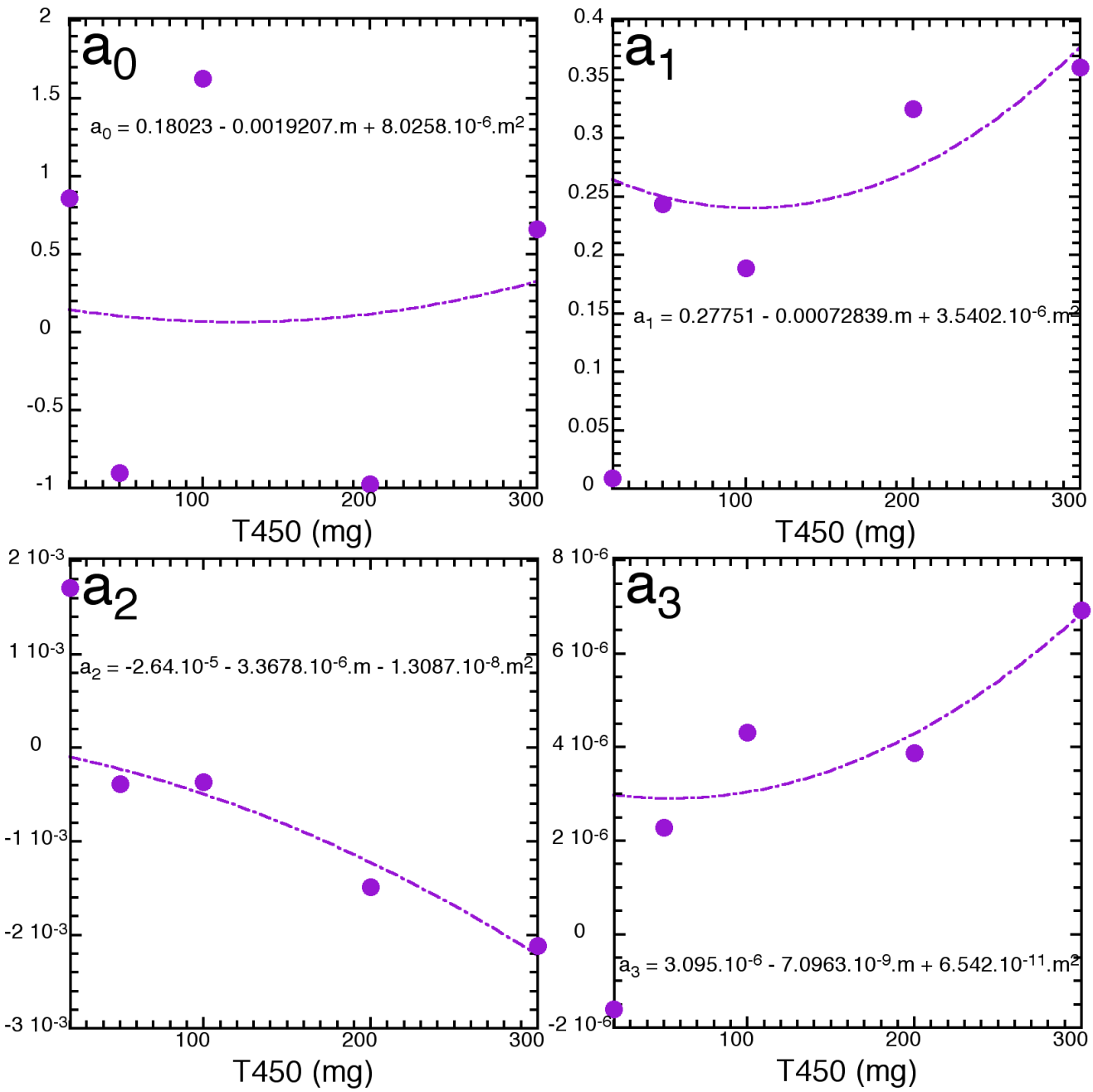


Figure S10: Values (dots) and 2nd order fit (dashed lines) of the polynomial parameters a_0(m) to a_3(m), with m the mass of T450, and the parameters a_0(m) to a_3(m) being the variable of the 3rd order degree polynomial [%(degrad) = a_0(m) + a_1(m).t + a_2(m).t^2 + a_3(m).t^3].

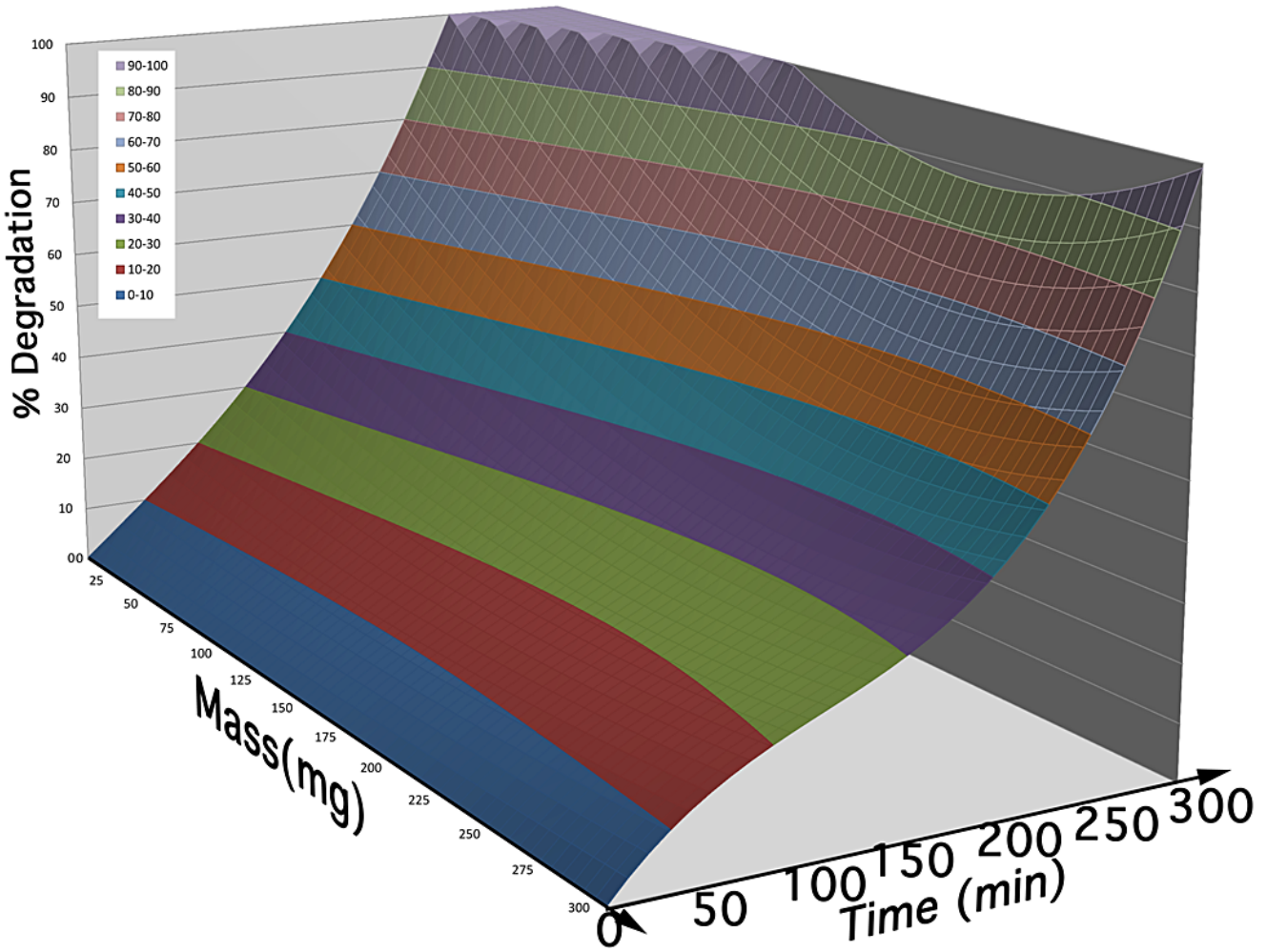


Figure S11: Modelling of the MB Degradation as a function of time (0 to 300 min) and mass (5 to 300 mg) , for the T450 sample.

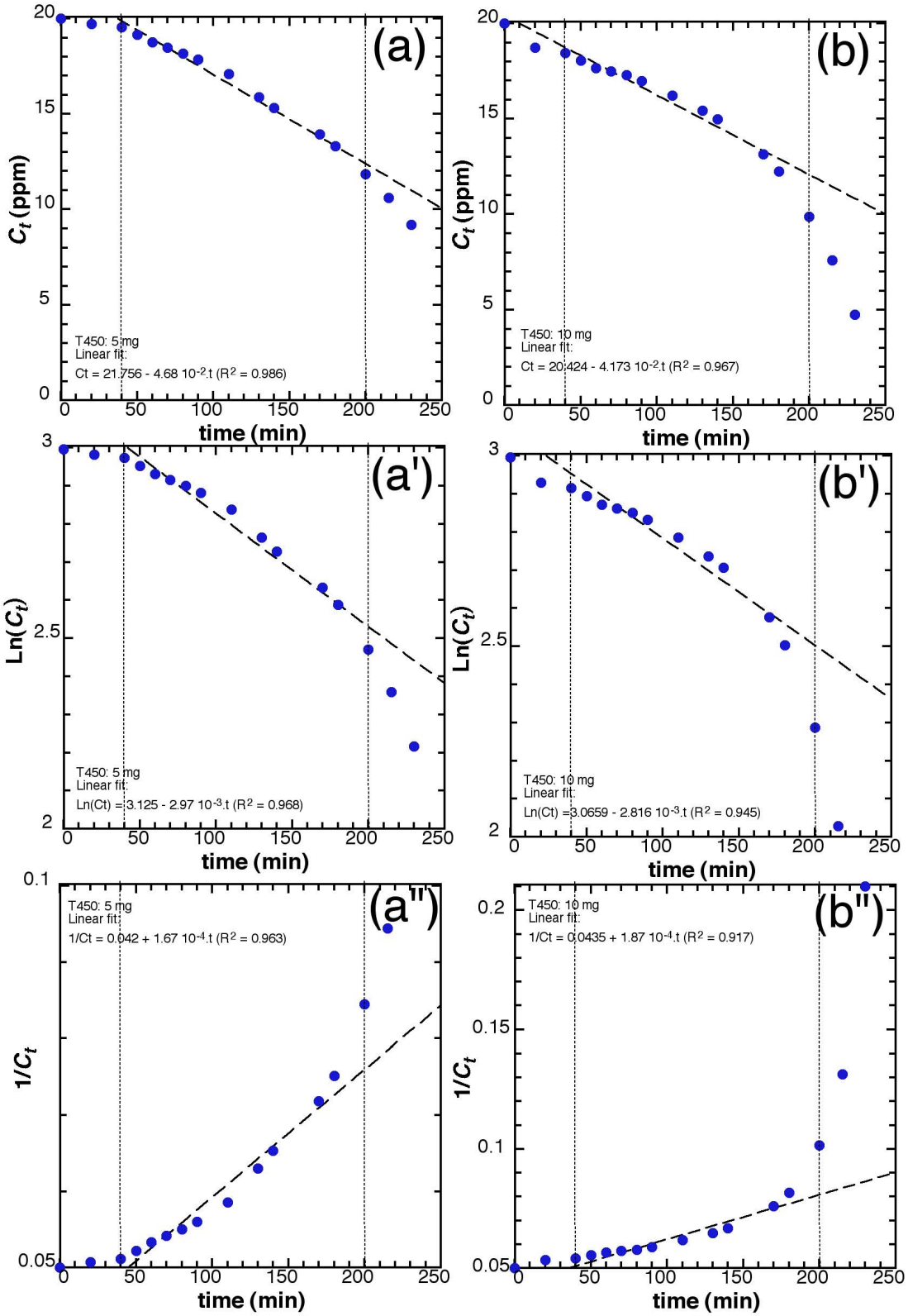


Figure S12-A: Linear fitting of the evolution of MB (in ppm) for the different kinetics models (Ct=f(t) - zero order; Ln(Ct)=f(t) - first order; 1/Ct=f(t) - second order) for 5mg of (a; a'; a"") and 10 mg (b, b', b") of T450.

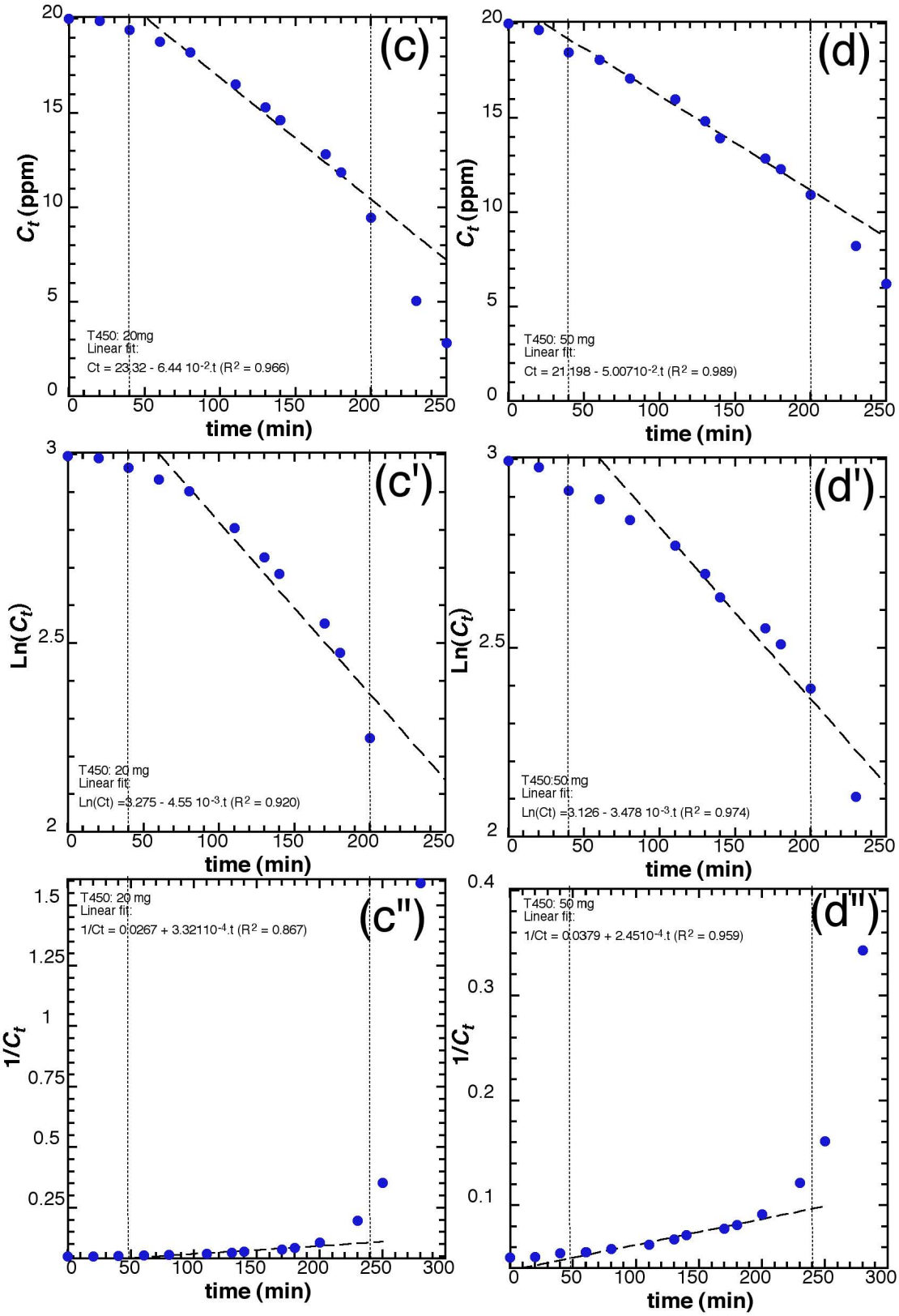


Figure S12-B: Linear fitting of the evolution of MB (in ppm) for the different kinetics models (Ct=f(t) - zero order; Ln(Ct)=f(t) - first order; 1/Ct=f(t) - second order) for 20mg of (c; c'; c"") and 50 mg (d, d', d") of T450.

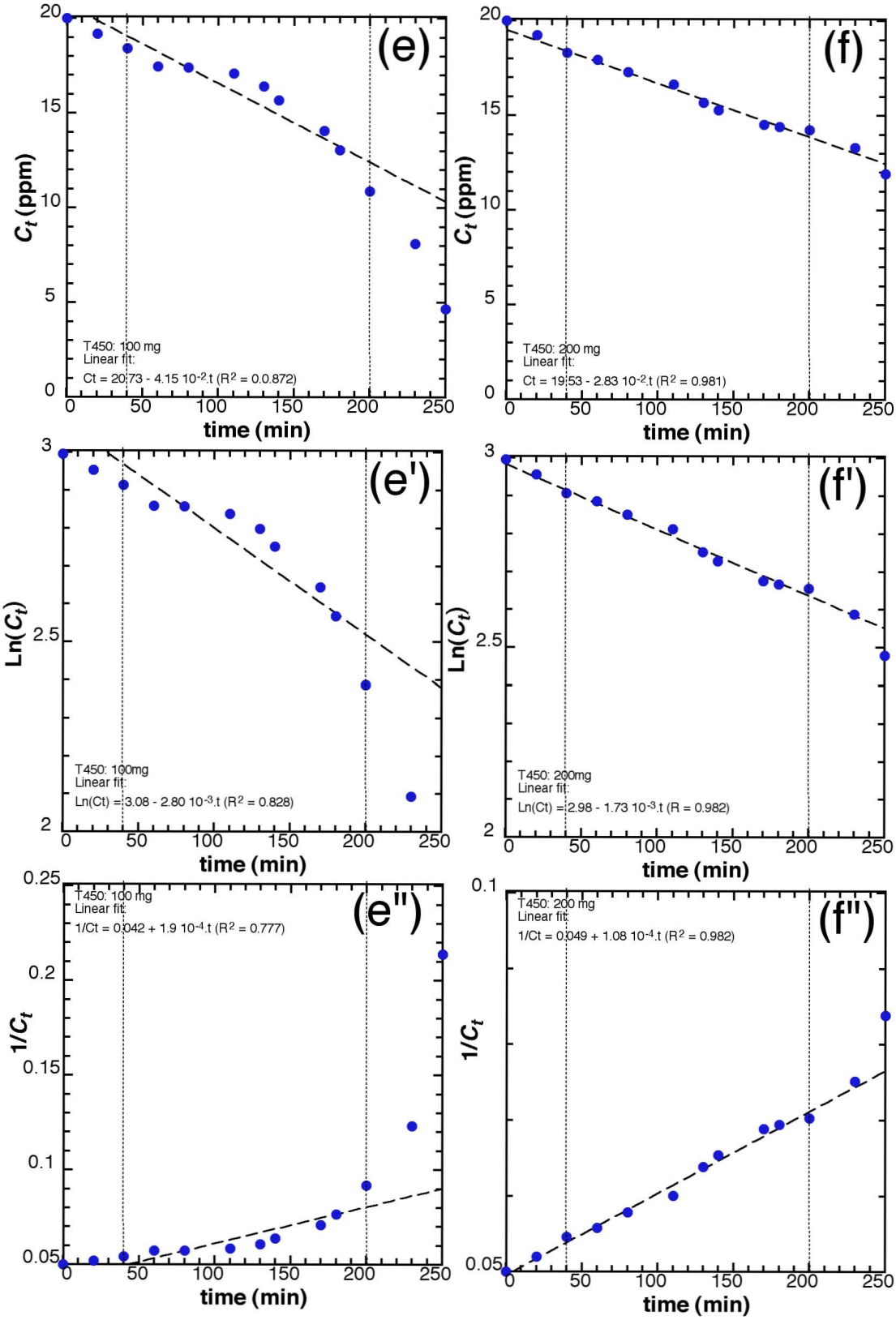


Figure S12-C: Linear fitting of the evolution of MB (in ppm) for the different kinetics models (Ct=f(t) - zero order; Ln(Ct)=f(t) - first order; 1/Ct=f(t) - second order) for 5mg of (e; e'; e"") and 200 mg (f, f', f") of T450.

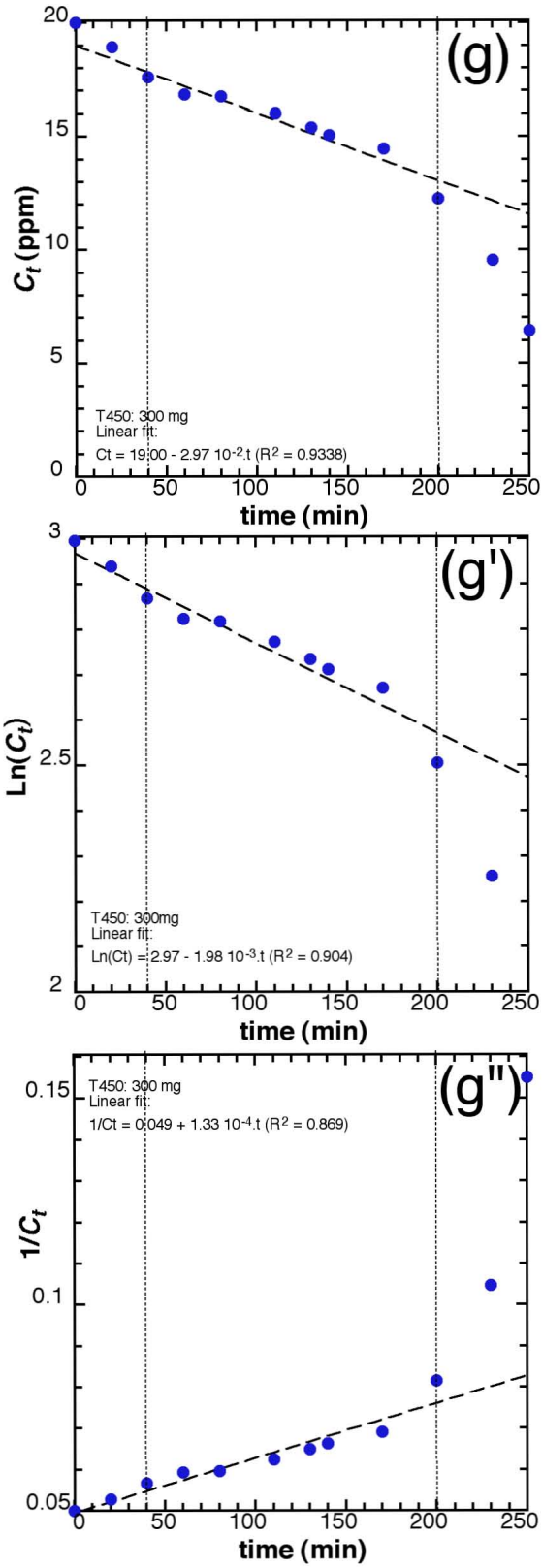


Figure S12-D: Linear fitting of the evolution of MB (in ppm) for the different kinetics models (Ct=f(t) - zero order; Ln(Ct)=f(t) - first order; 1/Ct=f(t) - second order) for 300mg of (g; g'; g"") of T450.

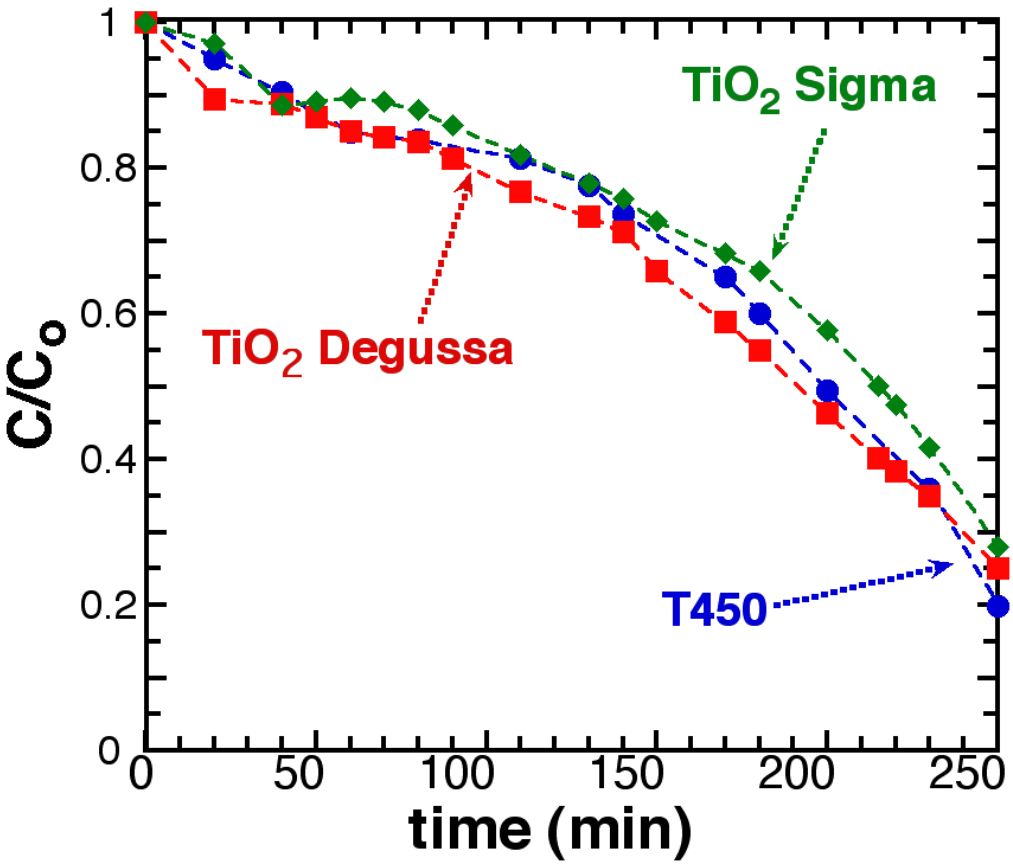
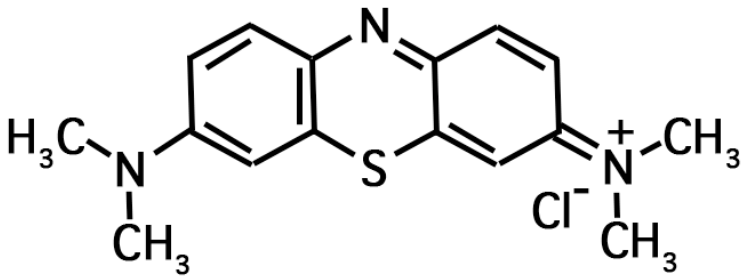


Figure S13: Comparison of the evolution of the concentration in Methylene Blue for TiO_2 Sigma, TiO_2 Degussa, and T450 (experimental conditions: 100 mG material in 25 mL, pH 6, MB: 20 ppm).



Scheme S1: Structure of Methylene Blue