

Photocatalytic Transformation of Triclosan. Reaction Products and Kinetics

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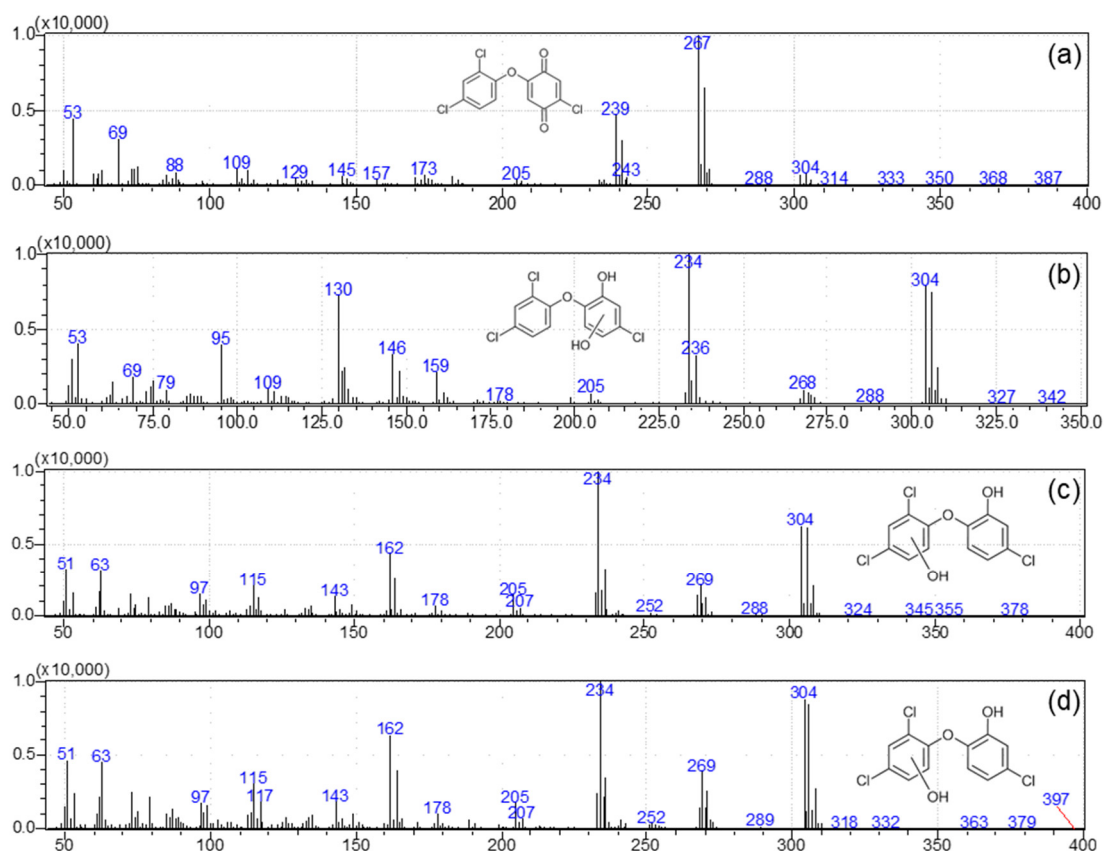


Figure S1. GC-MS spectra of the TCS derivatives: (a) TCS quinone, (b) hydroxylated TCS 1, (c) hydroxylated TCS 2 and (d) hydroxylated TCS 3

Table S1. 2,4-dichlorophenol kinetic constants reviewed in bibliography

2,4-DICHLOROPHENOL DEGRADATION			
Conditions	Kinetic equations and parameters		Reference
	Kinetic equations	k (min ⁻¹)	
[2,4-DCP] ₀ = 50 mg L ⁻¹ ; [TiO ₂] = 1.4 g L ⁻¹ ; V = 0.1 L; pH = 3-11; Hg lamp = 5.8 W, λ = 254 nm; Light intensity = 500 μW cm ⁻²	$-\frac{d24DCP}{dt} = \frac{kK [24DCP]}{1 + K [24DCP]}$ K = adsorption constant = 1.3 – 1.8·10 ³ L mol ⁻¹	k = 4.00-5.50·10 ⁻⁴ M h ⁻¹	1
[2,4-DCP] ₀ = 163 mg L ⁻¹ ; [TiO ₂] = 2 g L ⁻¹ ; V = 0.04 L; pH = 5.6; Hg lamp = 125 W; λ = 365 nm; Light intensity = 2.3·10 ⁻⁵ Einstein min ⁻¹	$-\frac{d24DCP}{dt} = \frac{K_1 K_2 [24DCP]}{1 + K_2 [24DCP]}$ K ₁ = reaction rate K ₂ = adsorption constant = 3.2·10 ³ L mol ⁻¹	K ₁ = 4.50·10 ⁻⁵ M min ⁻¹	2
[2,4-DCP] ₀ = 20 mg C L ⁻¹ = 45.2 mg L ⁻¹ ; [TiO ₂] = 0.1 g L ⁻¹ ; V = 0.8 L; pH = 6, Hg lamp = 125 W;	$\frac{d24DCP}{dt} = k_1 [24DCP]$	k ₁ = 3.28·10 ⁻² t _{1/2} = 22 min	3
[2,4-DCP] ₀ = 125 mg L ⁻¹ ; [TiO ₂] = 0.01-2 g L ⁻¹ ; V = 0.5-1.5 L; pH = 5.5; Solar simulator, (UV range up to 436 nm), Xe lamp = 1500 W	$\frac{d24DCP}{dt} = k_1 [24DCP] - k_2 [INTERM.]$	k ₁ = 1.20·10 ⁻² - 6.60·10 ⁻² k ₂ = 4.50·10 ⁻² - 9.00·10 ⁻³	4
[2,4-DCP] ₀ = 20 mg L ⁻¹ ; [TiO ₂] = 2 g L ⁻¹ ; V = 0.02 L; UV LED, λ = 365 nm; Light intensity = 8.55 × 10 ¹⁶ photon/s;	$\frac{d24DCP}{dt} = -k_{24DCP} [24DCP]$	k = 3.12·10 ⁻²	5
[2,4-DCP] ₀ = 25, 50, 75, 100 mg L ⁻¹ ; [TiO ₂] = 0.5 g L ⁻¹ ; V = 1 L; Solar simulator = 1000 mW cm ⁻²	$\frac{d24DCP}{dt} = -k_{24DCP} [24DCP]$	k (50 ppm) = 5.11·10 ⁻¹	6
TCS ₀ = 34.5 μM (10 mg L ⁻¹); TiO ₂ = 1.5 g L ⁻¹ ; V = 1 L; pH = 5.8; LED lamp (UV) = 35 W, λ = 365 nm	$\frac{dTCS}{dt} = -k_1 [TCS]$		This work
	$\frac{dHICs}{dt} = k_1 [TCS] - k_2 [HICs]$		
	$\frac{dDCP}{dt} = k_2 [HICs] - k_3 [DCP]$	k ₁ = 4.20·10 ⁻² k ₂ = 1.00·10 ⁻¹ k ₃ = 1.95·10 ⁻¹	
	$\frac{dLOCs}{dt} = k_3 [DCP]$	k ₄ = 2.92·10 ⁰	
	$-k_4 [LOCs]$		
	$\frac{dP}{dt} = k_4 [LOCs]$		

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