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ABSTRACT BOOK

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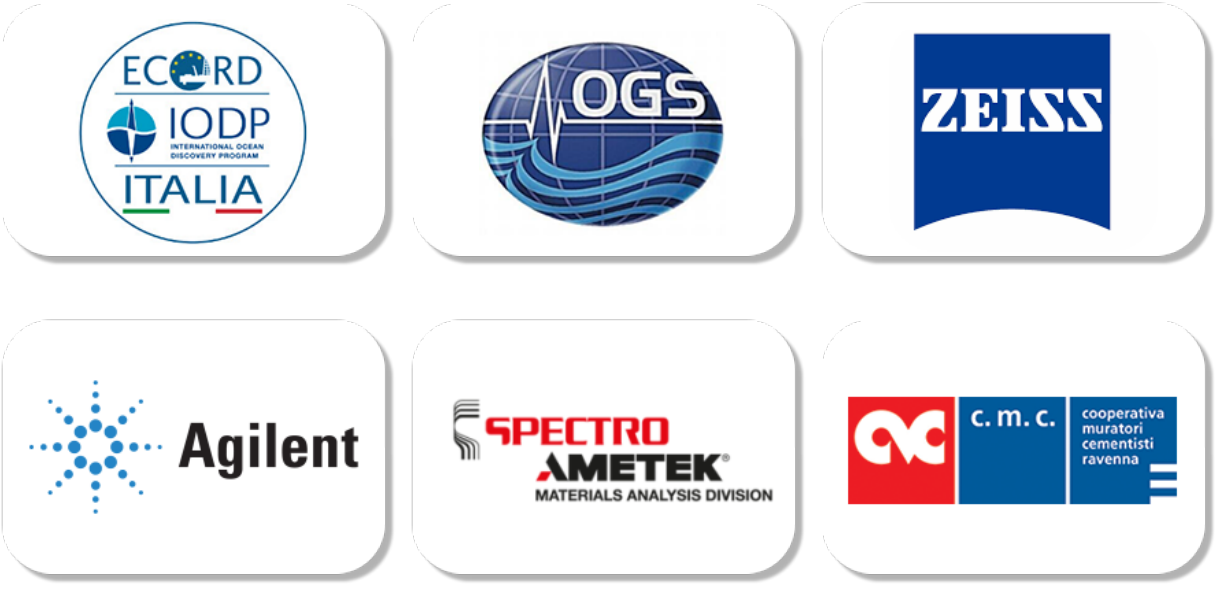

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Structural evidence of herbicide (2-ethyl-6-methylaniline) adsorption from aqueous solution in synthetic ZSM-12 zeolite

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Pesticides are include in the hazardous substances class and they are transferred into the environment through various pathways (*e.g.* surface runoff, subsurface and groundwater flows) (Levitan, L., 2000; Boithias, L. *et al*., 2011). According to the current directives regarding drinking water quality, an individual species of pesticide should be not present in the water body over the standard concentration of 0.1 g/l, while the overall concentration of different kind of pesticides should not exceed 0.5 g L^{-1} (EC, Directive 98/83/EC, 1998). The recent wide use of these pollutants in the intensive farming is causing of serious environmental problem due to the toxicity of pesticides for the animal and human health (Otero R. et al 2012). In particular, more attention should be done regarding the family of chloroacetanilides compounds and among them, Metolachlor (C15H22ClNO2), and their metabolites (*e.g.* 2-Chloro-N-(2-ethyl-6-methylphenyl)acetamide, 2-ethyl-6-methylaniline) are frequently detected in surface and subsurface water. For that reported above, this work is devoted to test the adsorption capability of synthetic ZSM-12 zeolite toward 2-ethyl-6-methylaniline ($C_2H_5C_6H_3(CH_3)NH_2$, labelled EMA). The removal from water solution of this degradation product of Metolachlor is evaluated through the use of combining chromatographic, thermogravimetric and synchrotron X-ray powder diffraction techniques. Specifically, the synchrotron radiation data was collected at the MCX beamline of Elettra-Synchrotron (Trieste) using a fixed wavelength (0.827Å). Initially, the structure of as synthesize material was characterized, by Rietveld refinemet, in order to verify the presence of the template 6-azonia-spiro-[5,5]-undecane as structure directing agent (ZSM-12-SDA). After calcination in order to remove the template, the ZSM-12 sample was loaded with EMA compound. The EMA concentration in the aqueous solution was determined by Headspace Gas Chromatography coupled to Mass Spectrometry (HS-GC-MS). The adsorption isotherm, determined using the batch method, highlight a very fast ZSM-12 adsorption kinetics. Afterward, the adsorption capacity of ZSM-12 was evaluated also with the Rietveld method. Based on the analysis of difference Fourier maps, EMA molecules was localised in the ZSM-12 channel and the refined occupancies suggest the adsorption of about 4 EMA molecules per unit cell, in very good agreement with the weight loss given by TG analyses (performed in air using an heating rate of 10°C/min, from room temperature up to 900 °C) and with the saturation capacity determined by the adsorption isotherms. To summarized, the obtained results (rapid kinetic combined with the good adsorption capacity) suggest that the ZSM-12 zeolite may be suitable to remove the tested pesticide from water and could represent a promising future candidate as an environmentally friendly alternative in the removal of acetanilides compounds.

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