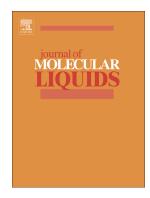
Accepted Manuscript

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PII:	S0167-7322(18)31563-0
DOI:	doi:10.1016/j.molliq.2018.04.100
Reference:	MOLLIQ 9003
To appear in:	Journal of Molecular Liquids
Received date:	23 March 2018
Revised date:	18 April 2018
Accepted date:	19 April 2018

Please cite this article as: Lorena Delgadillo-Velasco, Virginia Hernández-Montoya, Norma A. Rangel-Vázquez, Francisco J. Cervantes, Miguel A. Montes-Morán, Ma del Rosario Moreno-Virgen, Screening of commercial sorbents for the removal of phosphates from water and modeling by molecular simulation. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2018.04.100

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ACCEPTED MANUSCRIPT

Screening of commercial sorbents for the removal of phosphates from

water and modeling by molecular simulation

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Abstract

Eight commercial sorbents of different origin and nature were studied in the present work for the removal of phosphate from water using synthetic solutions and a wastewater from an anodizing company. The materials included activated carbons, bone char, catalytic carbon, natural silica, natural zeolite, a manganese(II) oxide composite and iron(III) hydroxide. These materials were characterized with different analytical techniques such as nitrogen adsorption isotherms at -196 °C, FT-IR spectroscopy, SEM/EDX analysis and X-ray diffraction. The adsorption studies were performed in batch systems. Iron(III) hydroxide was found the best sorbent, showing a maximum adsorption capacity of 193.75 mg/g at pH 7 in contrast with natural zeolite and silica, which registered very low adsorption values (2.92 and 4.17 mg/g, respectively). According to molecular simulation studies, the adsorption of phosphates from water on iron(III) hydroxide allowed the formation of the complex \equiv FePO₄H₂, with a Gibbs free energy of -21.38 kcal/mol, showing that it is possible to recover

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