A DFT Study on the Adsorption of Benzodiazepines to Clay Surfaces

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Benzodiazepines (BDZ) belong to the group of psychiatric substances which act on the central nervous system, having anxiolytic, sedative and hypnotic effects and is one of the most prescribed groups of pharmaceuticals throughout the world. These compounds are not exclusively used for human therapeutics, their prescription is also common in veterinary treatments for anxiolytic and appetite stimulation effects. Nowadays, there are several benzodiazepines under international control for therapeutic use. The widespread use of these compounds doesn't come without a cost and trace levels of it can now be found disseminated on the environment, what is a matter of ecological concern. In fact, over the last decade, there has been a significant number of studies reporting the occurrence of BDZ in environmental matrices, namely in wastewater treatment plants influents and effluents, surface waters and drinking waters [1-3]. Some of the more frequently detected BDZ include alprazolam, diazepam, lorazepam and oxazepam [1-3].

The main reason for the ubiquitous presence of BDZ in the environment is associated not only with the large use but also the generally low efficiency of conventional biological wastewater treatment to remove these pharmaceutical residues. It has been suggested that this inefficiency is due to the halogenated structure of these compounds that significantly reduces their susceptibility to biodegradation [4]. Adsorption processes are the most promising and cheap alternative for removal of these kind of organic xenobiotic from wastewaters. In recent years, inexpensive widely available materials have been investigated for the selection of efficient adsorbents that can make adsorption processes an attractive solution at reasonable costs. Among some of the adsorbents studied, clay-based materials have received some attention [5-7] due to their interesting properties such as the high cation exchange capacity, swelling properties and high specific surface areas. In particular for the treatment of wastewaters, these materials can overcome the limitations of biological processes, as used in conventional wastewater treatment. A better understanding of the interactions of these organic molecules with clay minerals may thus allow a more judicious selection of materials for water/wastewater treatment filters that present significant enhancements in the removal of BDZ.

In this work, electronic structure calculations based on the density functional theory (DFT) are presented on the interaction of two BDZ molecules (diazepam and alprazolam) with a periodic model surface of the vermiculite mineral. Geometry changes of the molecules upon adsorption were compared and the interaction energies with the surfaces were determined for a few different molecular orientations in order to understand the way these molecules interact with the clay surface and the essential factor governing the adsorption processes.

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