Computational screening of zeolites for the adsorption of selected pharmaceutical pollutants

Abstract

Molecular simulations have been used as a screening tool to identify promising zeolites for the removal of selected pharmaceutical pollutants. 40 zeolites with different structural and chemical configurations were studied. Galophosphate cloverite (CLO) of the chemical formula, $F_{24}Ga_{96}P_{96}O_{372}(OH)_{24}$, with pores of 20 rings and the lowest observed bulk density, showed exceptionally preferred adsorption of diclofenac [2-(2,6-dichlorophenyl)amino benzeneacetic acid), ciprofloxacin [1,3,7-Trimethylpurine- 2,6-dione] and chloramphenicol [2,2-dichloro-N-[(IR,2IR)-1, 3-dihydroxy-1-(4-nitrophenyl) propan-2-yl acetamide]. This selectivity was attributed to the geometry and structural composition of the cavities. We also investigated the most stable adsorbed compositions of the pollutants in the CLO zeolite. Our calculations show that diclofenac, ciprofloxacin and chloramphenicol molecules are adsorbed into the pores with adsorption energies of – 78.23, – 173.68 and – 84.46 kcal/mol respectively. Additional calculations were also made to obtain detailed information on desorbed products. It is seen that dechlorination is the most energetically preferred process compared to dehydrogenation and dehydroxylation.

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