

HIGH SILICA ZEOLITE Y FOR EMBEDDING SULFONAMIDE ANTIBIOTICS: AN AFFORDABLE MATERIAL FOR WATER CLEAN-UP AND DRUG DELIVERY

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Sulfonamide antibiotics are persistent pollutants of aquatic bodies, known to induce high levels of bacterial resistance. The adsorption of ten sulfonamides into a high silica zeolite Y with cage window sizes comparable to sulfonamide dimensions was studied in order to clean-up water polluted with sulfa drugs. At maximal solubility, nine sulfonamides were almost completely (>90%) and quickly ($t < 1$ min) removed from water by zeolite. With the exception of sulfanilamide which showed scarce affinity for zeolite Y (3% zeolite DW), the other sulfa drugs adsorbed at 26% zeolite DW on average. The presence of sulfonamides inside the cage was revealed by unit cell parameter variations and structural deformations obtained by X-ray structure analyses carried out using the Rietveld method on exhausted zeolite. For all the host-guest systems, the close vicinity of antibiotic aromatic moieties and their substituents with zeolite framework was evidenced by multidimensional and multinuclear SS-NMR and in situ FTIR spectroscopies and confirmed by ab initio computational modelling. Sulfonamides with the lowest steric hindrance (namely sulfadiazine, sulfathiazole and sulfapyridine) form H-bonded dimers inside zeolite cage. Multiple weak H-bonds and van der Waals type interactions between antibiotics and zeolite are responsible for the irreversible extraction from water of all the examined drugs. Lastly, the most stable tautomeric form of each antibiotic adsorbed into zeolite was identified. The sulfonamide amount loaded into zeolite Y is remarkably high to consider this material affordable not only for clean-up but also for drug delivery issue.

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