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<u>Entitled</u>

PH-CONTROLLED PREFERENTIAL BINDING OF CUCURBIT[7]URIL-COATED IRON-OXIDE NANOPARTICLES TO 6-MERCAPTONICOTINIC ACID FOR FLUORESCENT DETECTION OF CADMIUM IONS IN THE SOLID STATE

By

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<u>Abstract</u>

A host–guest complex of 6-mercaptonicotinic acid (MNA) and cucurbit[7]uril (CB7) was prepared and conjugated to γ -Fe₃O₄ nanoparticles (NPs) to detect toxic cadmium ions in water as a solid state sensor. The formation of an inclusion host–guest complex with CB7 was confirmed by UV–vis absorption and proton NMR spectroscopy. CB7 preferentially binds the protonated MNA form compared to the neutral form, demonstrated by a binding constant for the protonated form that is four orders of magnitude higher than the neutral form. An increase in the pK_a of MNA by 1.2 units was demonstrated after the addition of CB7, which further supports preferential binding between MNA and CB7. The NMR results confirm binding to cadmium via the carboxylic acid moiety. Stationary and time-resolved fluorescence results, in solution and in the solid state, indicate that cadmium and CB7 cause a blue shift in the MNA emission bands and extend its excited-state lifetime due to dissociation of the MNA dimer. In the solid state, switching the emission signals between Cd²⁺-MNA/CB7NPs (ON state) and MNAH⁺/CB7NPs (OFF state) was achieved by controlling the pH. An efficient, regenerable, and stable sensor device was fabricated for the sensitive and selective detection of Cd²⁺ in contaminated water samples.

Keywords: 6-mercaptonicotinic acid, cucurbit[7]uril, iron oxide nanoparticles, host-induced pKa shift, cadmium, time-resolved fluorescence, regenerable sensing, pH-controlled.

