

**SORBENT STUDIES OF HUMIC ACIDS
EXTRACTED FROM SOIL AND COAL SAMPLES
FOR THE REMOVAL OF URANYL IONS**

PhD (DISSERTATION)

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NOVEMBER, 2005

ABSTRACT

Humic acids were extracted from Htantabin soil sample and Kalewa coal sample, and characterization of these purified humic acids was done by using various techniques such as C, H, N analysis, XRD, FT-IR, SEM, nanoESI, MALDI-TOF-MS and TGA-DTA techniques. The amorphous character of the purified humic acids were revealed by XRD pattern. The typical functional groups of humic acid (-C=O, -OH, -COOH, -C=C-) were identified by FT-IR spectra.

Based on the elemental analysis of C, H, N data of the purified humic acids, the two types of different humic acids were found to have different compositions. Different nature of two humic acid samples were also deduced from MALDI-TOF-MS and nanoESI techniques. The molecular mass of humic acid from soil samples was found to be 1869 Daltons, whereas that of humic acid from coal samples was 2766 Daltons.

The sorption studies of uranyl ions with coal and soil humic acid samples were carried out on the effect of pH, initial concentration, contact time between uranyl ions and humic acid and dosage capacity of humic acids. These studies indicated that coal and soil samples exhibited different binding capacities towards uranyl ions. The removal percents of uranyl ions by coal and soil humic acid samples were found to be 91% and 82.5% corresponding to the optimum pH of 5-6 and 4-5 respectively. Coal humic acid sample possessed higher removal percent of uranyl ions and the sorption capacity than that of soil humic acid sample.

In the contact time study, variations of binding rate with time were found to be different between coal and soil humic acid samples. For soil sample, binding rate was maximum at 20 min and then decreased with time,

whereas binding rate of coal sample was maximum at 10 min and then decreased with time.

Characterization of uranyl-humate precipitated from uranyl ions and humic acid solutions were carried out by various techniques. FT-IR and FT-Raman spectra indicated the presence of asymmetric ($\nu_{as}(U=O)$) and symmetric ($\nu_s(U=O)$) stretching vibrations of uranyl ions in uranyl-humate samples. Upon co-ordination of humic acid onto uranyl ions, small frequency shift (8 cm^{-1}) in FT-Raman spectra was observed due to the weakening of $U = O$ after binding with humic acid. From TGA-DTA data, the more larger amount of decomposition and combustion took place for soil uranyl-humate than that for coal uranyl-humate.

In order to predict the binding between uranyl ions and humic acid, molecular modeling studies on humic acid monomer were done by using ChemOffice (2000 ultravision) software. The various types of energies were calculated by using conformational analysis. Other properties such as polarizability, cosmo solvation properties, partial charges and dipole moments were also calculated. The active sites that can co-ordinate to uranyl ions were also indicated by using the calculation of Mulliken partial charge distribution.

Regarding to the above findings even trace amount of uranyl ions concentrations ($< 0.2\text{ ppm}$) can be extracted by humic acid. Hence, humic substance which is cheap and readily available material is a potential source for the recovery of uranyl ions from waste materials or from minerals.

Keywords: *humic acid, uranyl ions, binding capacity, ChemOffice, conformational analysis, dipole moment, Mulliken partial charge, molecular modeling, MALDI-TOF-MS, nanoESI, FT-Raman.*