The Chemical Database Service Research Highlights

XANES fingerprinting of iodine species in nuclear waste - John Charnock

There are major environmental concerns with the use of nuclear fuels and associated technologies. One of the main areas of anxiety lies in the large amount of radioactive waste produced, and in the safe treatment and disposal of this. Radioactive iodine isotopes are retained in spent solvent (tributyl phosphate/odourless kerosine, TBP/OK) from nuclear fuel reprocessing, which causes problems in decontamination. The speciation of iodine in TBP/OK is difficult to determine due to the low concentration (ca. 40 ppm) in solution and the complexity of the solvent. XANES spectroscopy is element-specific and relatively independent of the sample medium, so is an ideal technique to use to investigate this speciation.

The iodine K-edge XANES spectrum of a spent solvent sample from a reprocessing plant was obtained and compared with the XANES spectra of eight reference compounds containing iodine in oxidation states from -1 to +7. This comparison suggests that the most likely state of the iodine in the solvent is as an organoiodide species, although it is possible that smaller amounts of other species may also be present [1]. This knowledge may help in the design of a process for removing the iodine from the solvent.

The CDS databases ICSD and CSSR were used to identify structurally characterised iodine species with different coordination environments and oxidation states for use as reference compounds in this study. Full X-ray absorption spectra (comprising XANES and EXAFS) were collected for these compounds and the structural data from the CDS databases were used to compare with the EXAFS analysis results. This provided a check that the EXAFS interpretation is reliable and aided the determination of the coordination environment of the iodine in the TBP/OK solutions

[1] W. A. Reed, I. May, F. R. Livens, J. M. Charnock, A. P. Jeapes, M. Gresley, R. M. Mitchell and P. Knight, *Journal of Analytical Atomic Spectroscopy*, 2002, **17**, 541-543.