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A Solid-State NMR Study of the Complexation of 109Cd with Isosaccharinic Acid

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The binding of 109Cd to isosaccharinic acid using advanced solid state NMR techniques was examined. The complexes, as well as ISA itself, were analysed at 3 different pHs (7, 10 and 13). Various solid-state NMR techniques were used. CP-MAS provided C-13 spectra of the complexes and the related dipolar dephasing method helped to determine the assignment of CH and CH2 groups. Slow sample spinning provided sufficient spinning side bands to allow the extraction of the CSA values. Experimental compared with calculated techniques were also carried out using Gaussian, Herzfeld Berger and Simpson programmes to look at differences in the spectra but also the CSA of the nuclei in the complex. The spectra of ISA at the various pHs were obtained first. Spectra were then obtained for the metal-ligand complexes. These spectra have enabled more detailed theories to be drawn up on the nature of the binding of radionuclides to polyhydroxylated carboxylic acids at varying pH.

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