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EXAFS AND XANES SPECTROSCOPY OF GA AND CA IN BONE AND RELATED MATERIALS. Lawrence R. Bernstein, Center for Materials Research, Stanford University, Stanford, CA 94305-4045; and Richard S. Bockman, Memorial Sloan-Kettering Cancer Center, New York, NY 10021.

Gallium is concentrated by living bone and can be very effective in preventing the loss of bone mineral both *in vivo* and *in vitro*. Human and animal studies have found that gallium nitrate treatment halts accelerated bone resorption due to bone cancer, normalizes cancer-related hypercalcemia, and may be applicable to a wide range of degenerative bone diseases including osteoporosis. Gallium *in vivo* concentrates mainly in the parts of bone where new hydroxylapatite (HA) is added, particularly the epiphyseal plates in the metaphyses.

In this investigation, long bones (femurs, tibia, and humerii) from gallium-treated and untreated rats were studied by EXAFS and XANES spectroscopy using a fluorescence detector at SSRL. Material from the diaphyses (shafts) and metaphyses (ends) were studied separately. Diaphyses from the Ga-treated rats contained about 275 ppm Ga and the metaphyses contained about 360 ppm Ga (by atomic absorption analysis). Ga and Ca spectra were obtained on these materials. Ca spectra were also obtained on synthetic HA, brushite, octacalcium phosphate, and whitlockite. Ga spectra were also obtained on beta gallium oxide, gallium nitrate nonohydrate, and gallium acetate.

Gallium nitrate nonohydrate and gallium acetate were found to have Ga octahedrally coordinated to oxygen with an average bond length of 2.00(1) A. Ga in all the bone samples was found to be coordinated to O with r=1.91(1) A; no other shells of neighboring atoms were seen in the Fourier transforms of the EXAFS data. The results suggest that about 54% of the Ga is in tetrahedral coordination (r=1.828 A) and 46% in octahedral coordination (r=2.005 A). It is highly unlikely that significant Ga substitutes for Ca in HA (r=2.37 A). It is likely that most of the Ga is in Ga phosphates (tetrahedral Ga), with much of the rest being adsorbed or in other compounds. This agrees with other experimental results that show Ga to rapidly precipitate from serum-like solutions as insoluble Ga phosphates, which then act as nucleii for rapid HA precipitation. Experiments also show Ga to become adsorbed on HA, slowing both the crystallization and dissolution of the HA. This combination of effects could explain the observed stabilization of bone mineral observed in gallium nitrate treated individuals.