ABSTRACT

Highlights and Breakthroughs:

Molecular water in nominally unhydrated carbonated hydroxylapatite: The key to a better understanding of bone mineral

The exact nature of the mineral component of bone is not yet totally defined, even though it is recognized as a type of carbonated hydroxylapatite. It is rather remarkable that such fundamental natural material, which forms all hard parts of the human body except for small portions of the inner ear, is not well understood. Authors Jill Pasteris, Claude H. Yoder, and Brigitte Wopenka have undertaken detailed and truly painstaking experiments to characterize bone material and shed light on its relationship to hydroxylapatite. The authors very effectively demonstrate, through through Raman spectroscopic and thermogravimetric analysis of 56 synthetic samples of carbonated apatite containing from 1 to 17 wt% CO_3, that bone material is not simply carbonated hydroxylapatite, but instead a definable mineralogical entity, a combined hydrated-hydroxylated calcium phosphate phase of the form $Ca_{10-x}[(PO_4)_{6-x}(CO_3)_x](OH)_{2-x}$•nH2O, where n~1.5. They hypothesize that water molecules keep the apatite channels stable even when 80% of the hydroxyl sites are vacant (typical in bone apatite, in contrast to hydroxylapatite), and hinder carbonate ions from substituting for hydroxyl ions in the channels, thus regulating chemical access to the channels. The results of this study are extremely important in many fields, and will be of particular interest to those in medicine who study diseases of the bone.

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Molecular water in nominally unhydrated carbonated hydroxylapatite: The key to a better understanding of bone mineral

As noted by the authors, the exact nature of the mineral component of bone is not yet totally defined, even though it is recognized as a type of carbonated hydroxylapatite. It is rather remarkable that such fundamental natural material, which forms all hard parts of the human body except for small portions of the inner ear, is not well understood. Authors Jill Pasteris, Claude H. Yoder, and Brigitte Wopenka have undertaken detailed and truly painstaking experiments to characterize bone material and shed light on its relationship to hydroxylapatite.

The authors very effectively demonstrate that bone material is not simply carbonated hydroxylapatite. The study addresses the hydration state of bone mineral through Raman spectroscopic and thermogravimetric analysis of 56 synthetic samples of carbonated apatite containing from 1 to 17 wt% CO_3, synthesized in H_2O or D_2O. The results of the study are rather remarkable; their TGA results quantitatively document that, regardless of the concentration of carbonate in the structure, all carbonated "hydroxylapatites" contain ~ 3 wt% of structurally incorporated water in addition to adsorbed water. The authors confirmed by spectroscopic methods that natural bone mineral also contains structurally incorporated molecular H_2O.

The authors' data support a model in which water molecules densely populate the apatite channels regardless of the abundance of hydroxyl vacancies. They hypothesize that water molecules keep the apatite channels stable even when 80% of the hydroxyl sites are vacant (typical in bone apatite, in contrast to hydroxylapatite), and hinder carbonate ions from substituting for hydroxyl ions in the channels, thus regulating chemical access to the channels. As they note, their *results show that bone apatite is not a "flawed hydroxylapatite," but instead a definable mineralogical entity, a combined hydrated-hydroxylated calcium phosphate phase of the form* $Ca_{10-x}[(PO_4)_{6-x}(CO_3)_x](OH)_{2-x}\bullet nH2O$, *where n~1.5. Water is therefore not an accidental, but rather an essential, component of bone mineral and other natural and synthetic low-temperature carbonated apatite phases.*

The results of this study are extremely important in many fields, and will be of particular interest to those in medicine who study diseases of the bone.