THERMALLY-INDUCED CHANGES OF CARBONATE STRUCTURE IN BIOLOGICAL HYDROXYAPATITE AS STUDIED BY EPR AND ENDOR

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S u m m a r y

Changes of the carbonate structure in tooth enamel hydroxyapatite under annealing in the temperature interval $T_{\rm ann}$ = 20–1000 °C are studied by electron paramagnetic resonance (EPR) and electron nuclear double resonance (ENDOR). In our studies, CO_2^- radicals induced by γ-irradiation after the annealing of specimens are used as a probe. The lineshape of EPR spectra and proton (^{1}H) and phosphorus (^{31}P) ENDOR spectra, as well as their thermally induced modifications, are analyzed and explained. It is shown that the general tendency under the annealing of specimens is the escape of carbonate from biohydroxyapatites and its simultaneous transformation from type B into type A at $T_{\rm ann} > 700$ °C. Specific features of carbonate escape from biohydroxyapatite at $T_{\rm ann}$ = 400 °C are explained by the formation of localized CO_2 molecules in apatite. The results obtained correlate with the data of IR and NMR studies of tooth enamel, as well as with the EPR and ENDOR spectra of CO_2^- radicals in synthetic hydroxyapatites.