

Optics and Spectroscopy (English translation of Optika i Spektroskopiya) 2014 vol.116 N5, pages 715-720

A study of hydroxyapatite nanocrystals by the multifrequency EPR and ENDOR spectroscopy methods

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Abstract

Specimens of powders of hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$) with average crystallite sizes in the range of 20-50 nm synthesized by the wet precipitation method have been investigated by the multifrequency (9 and 94 GHz) electron paramagnetic resonance (EPR) and electron-nuclear double resonance (ENDOR) methods. In specimens subjected to X-ray irradiation at room temperature, EPR signals that are caused by nitrogen compounds have been observed. Numerical calculations performed in terms of the density functional theory show that the observed EPR signal is caused by the occurrence of paramagnetic centers, the structure of which is NO_3^{2-} and which replace the positions of PO_4^{3-} in the hydroxyapatite structure. © 2014 Pleiades Publishing, Ltd.

<http://dx.doi.org/10.1134/S0030400X14050051>
