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SOLID STATE NMR SPECTROSCOPY STUDY OF CALCIUM PYROPHOSPHATE ($\text{Ca}_2\text{P}_2\text{O}_7$) POLYMORPHS EXPOSED TO X-RAY RADIATION

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Calcium phosphates (CaPs) are a versatile family of materials most widely used as bone graft substitutes and for targeted drug delivery in biomedical fields [1], in creation of sensors for direct detection of phosphate in aqueous solutions [2], in water purification for heavy metals [3], etc. CaPs are known for their biocompatibility, they are also easily and inexpensively produced, are safe, and can be relatively easily certified for clinical use. In the medical field, calcium orthophosphates such as hydroxyapatite (HA, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$), tricalcium phosphate (TCP, $\text{Ca}_3(\text{PO}_4)_2$), and amorphous calcium phosphate (ACP) are frequently utilized. Recent studies on biomaterials showed the potential of the use of calcium pyrophosphate (CPP, $\text{Ca}_2\text{P}_2\text{O}_7$) for biomedical applications [4]. We studied α -CPP, β -CPP and γ -CPP polymorphs.

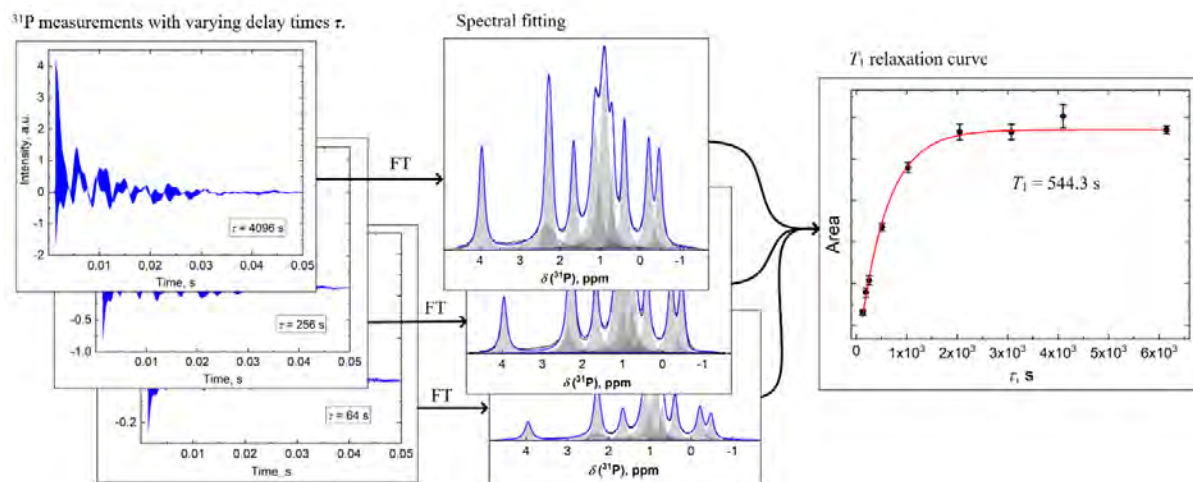


Fig. 1. Visualized procedure of the T_1 relaxation measurement. Left – acquired free induction decays (FID) of the samples. Middle – after Fourier transform (FT) peaks were approximated by theoretical curves. Right – first peak's (3.95 ppm) T_1 relaxation curve and fitting by using Eq. (1) approximation.

$$I(\tau) = I_0 \cdot \exp\left(-\frac{\tau}{T_1}\right) \quad (1)$$

To study CPPs, solid-state nuclear magnetic resonance (NMR) was used. Spin-lattice (T_1) relaxation times were measured using the saturation recovery method. Radiation-exposed CPP samples showed reduced relaxation times. For overlapping peaks spectral fitting using Gauss, Lorentz or Voigt theoretical spectral lines were performed. The overlapping peaks positions were referenced from [5] article. By examining the dependence of relaxation time by exposure time, the structural integrity of CPP polymorphs was evaluated.

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