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CHEMOMETRICS FROM THE CALCIUM PHOSPHATES BY FOURIER TRANSFORM INFRA RED SPECTROSCOPY

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Our study will investigate, how effective differentiation of Fourier transform infrared (FTIR) spectra can be done by FTIR processing techniques and chemometrics. FTIR spectroscopy is an important tool in the analysis of calcium phosphate. A major advantage of FTIR spectroscopy is, that spectra can be obtained from almost any physical state of sample (solutions, suspensions, powders). This research includes following steps of study:

- Sampling and Spectral recording.
- Pre-processing (normalization, baseline correction; "translation") of spectra.
- Spectral processing with different software for analysis of spetra.
- Statistical analysis/Chemometrics (such as Principal component analysis (PCA), Factor analysis (FA), Pearson product-moment correlation coefficient (PPMCC) and Cluster analysis (CA). Cluster analysis uses Euclidean and Hierarchical methods).

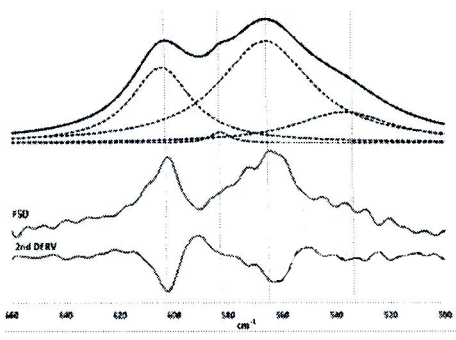

Fig. A graph showing FTIR spectra curve fitting, self-deconvolution and second derivative

In this research we found:

- Deconvolution of spectra improves understanding of materials that show complex FTIR spectra.
- PCA, CA proves to be valuable tool for analyses of FTIR spectra for research of testing methods and materials
- Modern software supports an efficient and intuitive analysis of sophisticated statistical analysis.

References:

[1] Li J., Hibbert D. B., Fuller S., Vaughn G., *Chemometrics and Intelligent Laboratory Systems*, **2006**, vol. 82, 50-58.

[2] Gu C., Katti D. R., Katti K. S., *Spectrochim. Acta A Mol. Biomo.l Spectrosc.* **2013**, *103*, 25-37.