H99 Quantifying Heat Exposure of Osseous Material Utilizing Novel FTIR Peak Ratios

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After attending this presentation, attendees will have gained an understanding of how indices calculated from Fourier Transform Infrared Spectroscopy-Attenuated Total Reflectance (FTIR-ATR) absorption peaks can give vital information regarding the burn temperature and exposure time of bone that has been subjected to fire.

This presentation will impact the forensic science community by reforming traditional methods of predicting heat exposure of bone and significantly improving the rate of accurate temperature prediction in experimental burnings from 19% using the traditional method to 82% when incorporating the new ratios.

Bone can reveal insightful information about an individual's life and circumstances of death. Professionals of various disciplines have an interest in understanding the changes bone undergoes when subjected to fire, be they archaeologists investigating ancient burial practices or forensic personnel confronted with the reconstruction of a scene of accident or crime.

Traditionally, only the so-called Crystallinity Index (CI), which is defined by the splitting of the two absorption peaks at 605 and 565cm^{-1} when using spectroscopy as a mean of analysis, has been used to gain an understanding of the heat exposure bone has undergone. The higher the exposure temperatures, the more ordered the bone structure becomes, exhibiting larger hydroxyl apatite crystals; however, this trend is reversed at temperatures above 800°C, due to the complete loss of all organic components and a shift in the elemental ratios. The consideration of the entire FTIR spectrum, therefore, lends itself for a better understanding of heat-induced changes to the bone matrix.

The present study investigated the use of new absorption peaks for the determination of burning temperatures and duration. Research was carried out using defleshed rib bones of domestic sheep (*Ovis aries*) which were experimentally burned in a furnace for 45 min at temperatures between 50°C and 1100°C in 50°C increments. For each temperature, two bones were burned, each of which was sampled nine times, resulting in a total of 18 samples per temperature. These ground samples from the periosteal surface of the bones were then analyzed on a Nicolet 5700 FTIR-ATR at an optical range of 2000cm^{-1} to 400cm^{-1}. Principal Component Analysis (PCA) was performed on all possible absorption peak ratios of the normalized spectra and determined the following ratios to be the most powerful to discriminate between different burn temperatures: CI=(565cm^{-1}+605cm^{-1})/595cm^{-1}, CO/P=1650cm^{-1}/1035cm^{-1}, CO/CO_3=1650cm^{-1}/1415cm^{-1}, CO_3/P=900cm^{-1}/1035cm^{-1}, Phosphate High Temperature (PHT)=625cm^{-1}/610cm^{-1} as well as the Line Width, which is defined as the full width at half the maximum of the phosphate peak at 1035cm^{-1}.

PCA also determined that combinations of different ratios are appropriate for different temperature ranges; low temperature burnings (<400°C) are best identified using C/P, CO/CO_3, CO_3/P, CO/P, and the Line Width, temperatures in the middle ranges (400°C –700°C) by the CI and the Line Width and high temperature ranges (>700°C) by the PHT as well as the C/P ratio.

Subsequently, Linear Discriminant Analysis (LDA) was performed based on the calculated indices of each of the spectra. It was found that the rate of accurate temperature prediction within a range of +/- 50°C was 82% in experimental burnings, which is a significant improvement when compared to the 19% accuracy achieved when solely using the CI, as it has commonly been done in the past. These findings are very promising for the advancement of burned bone analysis.

Burnt Bone, FTIR, Crystallinity Index