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Data Article

FTIR spectroscopy and VSC-based colour assessment dataset for comparative analysis of cremated bones

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ABSTRACT

The data presented in this article derives from archaeological cremated bones excavated in 2014–2015 at Aakre Kivivare tarand cemetery, S Estonia. The material covers bone fragments of different colours to be assessed visually, using Video Spectral Comparator (VSC) and analysed comparatively with Fourier Transform Infrared Spectroscopy (FTIR) to determine the structural and compositional changes in the thermally altered bone and implications of the latter in bone colouring.

The dataset comprises FTIR spectra measurements, colour spectra measured with VSC and visually assessed colour of human and animal bones chosen for the study. This dataset is expected to be a comparative source for determining archaeological cremated bone colour induced by heat-related changes in the bone microstructure, supporting the visual estimations of temperature-based cremation practices in archaeological and forensic bone material in the future.

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Specifications Table

Subject	Archaeology (osteology)
Specific subject area	Analysis of cremated archaeological and forensic human remains.
Type of data	Raw Table, Processed Table, Raw Image
Data collection	The data were collected by visual assessment, Video Spectral Comparator (VSC) and analysed with Fourier Transform Infrared Spectroscopy (FTIR)
Data source location	The archaeological material was excavated from Aakre Kivivare tarand cemetery in 2014 and the material is stored in the archaeological collections of the University of Tartu. The visual assessment of the bones was undertaken in 2015 in Bradford University and FTIR and VSC analyses in 2015 in Teesside University.
Data accessibility	Repository name: Zenodo Data identification number: 10.5281/zenodo.13120969 Direct URL to data: https://doi.org/10.5281/zenodo.13120969
Related research article	-

1. Value of the Data

- These data provide the characteristics of cremated bone with three different methods that can be used to interpret the cremation temperature affecting the osseous material.
- These data offer insight to the cremation practices and can be used to complement the interpretation of cremated human remains, both archaeological and modern.
- These data provide insight on the comparison of visual and measured spectral assessment and can aid in overcoming observer bias.
- The combination of these two relatively simple and cheap methods (FTIR and VSC), that are accessible in terms of instrumental cost and interpretative resources, has been scarce and should be acknowledged more widely.
- These data can be compared with other data of cremated osseous material regardless of spatio-temporal context.

2. Background

Visually detectable bone colour variations are the first traits suggesting cremation and indicating the duration and temperature of the pyre [1,2]. The most widely used approach for determining those processes in archaeological material is visual macroscopic assessment of the bone colour and physical attributes referring to pyre conditions and differential oxygen flow [1,3,4]. However, it has been outlined that visual macroscopic assessment is always subject to observer bias [5], and thus objective assessment criteria for chemical constituency of the bones needs to be developed. In archaeological collections, the vast quantity of the material, unfortunately, sets limits to the use of machinery for all the fragments, therefore it is advised that macroscopic and microscopic analyses should be employed holistically rather than exclusively [6,3]. FTIR characterises chemical and structural components of the bone and gives insight what changes the bone has undergone [7]. Experimental work has correlated cremation temperatures with these chemical and structural changes in the bone material [8]. FTIR has been used as an analytical tool to investigate the decomposition of the cremated bones for some time now [8,9]. VSC is mostly used in forensic contexts to explore written or printed documents, particularly regarding forgeries [10].

3. Data Description

These data include FTIR and VSC spectra of human and animal bone fragments from an Early Iron Age (2nd–5th cent AD) tarand cemetery in southern Estonia, Aakre Kivivare [11]. Samples

Table 1
Example of the table “Aakre samples, determination”.

Sample number	Human or animal	Bone fragment	Specific determination
12	Human	long bone	upper extremities or fibula
21	Human	long bone	-
33	Animal	long bone	-
…			

were collected during archaeological excavations by Anu Lillak (AL) and Maarja Lillak [12], assessed and sampled by AL, full osteological assessment is available in Estonian [13]. The samples were chosen to represent different colour hues and contain fragments with diagnostic features as well as material that is determined merely as “a long bone fragment”. The samples were transported to Teesside University by AL where she conducted the spectra measurements on FTIR and VSC.

The data comprises two MS Excel tables “Aakre samples, determination”, “Aakre colours, visual determination” giving context to the measurements in the folder “Aakre spectra”. The folder “Aakre spectra” includes two sub-folders “Aakre VSC” and “Aakre FTIR” containing the spectral measurement results of the corresponding devices.

The data in the table “Aakre samples, determination” is organized into four columns: “Sample context number”, “Human or animal”, “Bone fragment” and “Specific determination” (Table 1). This table characterises the sampled bones as accurately as it was morphologically possible. All the analysed bones, except sample 725 (a distal phalanx), were extremely fragmented. 10 of the sampled bones belonged to animals, 56 to humans and for 12 samples it was not possible to determine the origin. For 45 samples it was possible to specify the body part where the bone was from, but the remainder were anonymous long bone fragments.

The data in the table “Aakre colours, visual determination” is organized into three columns: “Sample context number”, “Visually assessed colour”, and “Comment”. It includes the visually assessed colours of the bones according to Holck [4] and Wahl [14]. The representation of different colours in the dataset is illustrated in Fig. 1.

The data in the “Aakre FTIR” folder includes the measurements of the spectra by FTIR-ATR and the data is in .csv and .SPA files that can be analysed and visualized with different software, e.g. Excel, R, Omnic (Fig. 2.).

The data in the “Aakre VSC” folder contains individual colour spectra measurements by VSC on each fragment in .csv form. Additionally, VSC provided a .JPG photo of each analysed fragment with the metadata on the photo under the image and in the corresponding .set file. This folder also contains a table “Aakre table, all VSC together” where all the VSC spectra are copied into one table, the first row states the “context number”, second row states the “visually assessed colour of the fragment” and the rest of the table contains the absorption spectra at different wavelengths.

The datasets are linked with unique reference numbers referring to the bone sample context number the material came from. For the spectra, the context number is in the name of the file and in MS Excel sheets, the context is found in the first column or row of the table.

4. Experimental Design, Materials and Methods

The data is based on the analysis of 78 samples of cremated archaeological human and animal bones from an Early Iron Age cemetery in southern Estonia, Aakre Kivivare, tarand cemetery dating 2nd–5th centuries AD (Fig. 3).

First, the bones were analysed visually, the fragments’ location in the skeletal system was determined based on their morphology and any characteristic traits on the bones were recorded. Since the bones are from an archaeological sample, the exact duration and temperature of the cremation are unknown. However, as these factors are correlated with both visual [3,4,14] and

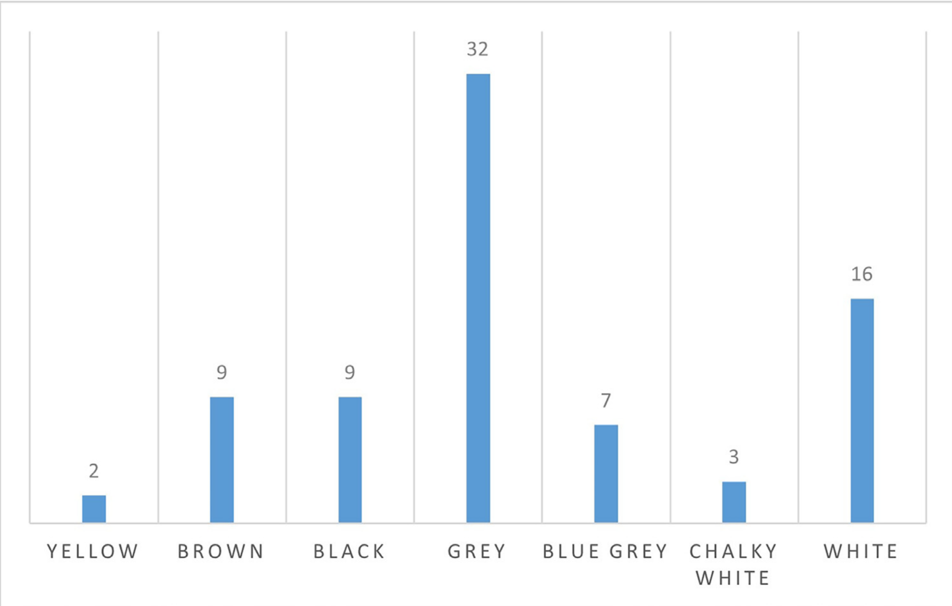

Fig. 1. Counts of the visually assessed colours among the sample material.

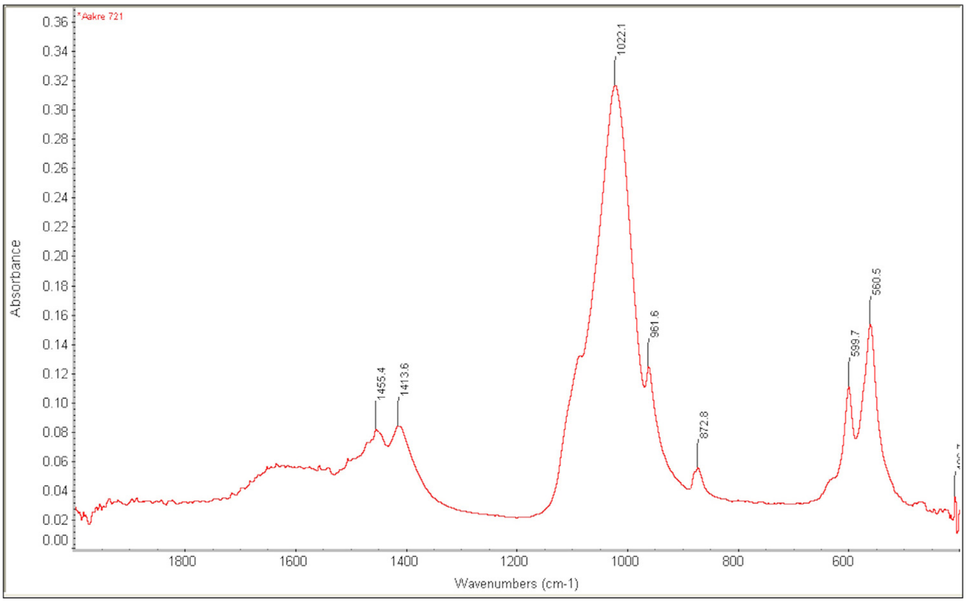

Fig. 2. FTIR spectrum of bone fragment from context 721 visualised with Omnic software and the peak values pointed out on the graph.

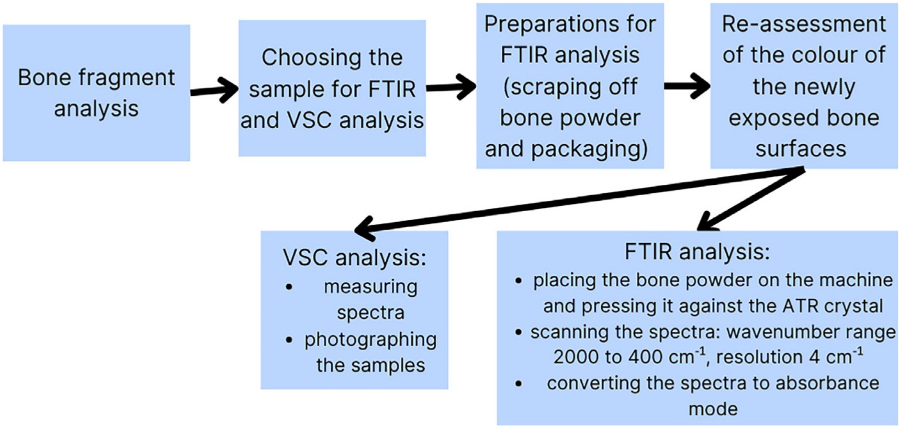

Fig. 3. The schematic description of the sampling process and analyses.

molecular [3,7–9] changes in the bone material, all bones were visually assessed, and some were further analysed using FTIR.

The bones' colour was visually assessed and documented in combination with methods by Holck [4] and Wahl [14]: yellow, brown, black/sooted, grey, blue grey, chalky white (in cases where the bone surface was soft), white. A characteristic sample, comprising approximately 3 % of the material, was selected for further analysis using FTIR and VSC. This sample included bone fragments of all the recorded colours, with a higher representation of the more common colours (grey and white) aiming to receive a generalizable overview of the material. While selecting the sample, care was taken to ensure that bones with characteristic features were not affected to the extent that they lost their morphological information. As the individual bones exhibited different colours as well as potentially differential exposure to heat, the visual estimation was focused on the area of the bones that was later analysed with VSC and FTIR. For the FTIR analysis, a small amount of material was scraped off the bone fragment's edge with a clean scalpel. The powder was packaged in small glass containers and labelled. In some cases, the surface and the internal colour of the bone differed in some cases as can be observed in the photos stored in the "Aakre VSC" folder.

The colour spectrum of the area was measured with Video Spectral Comparator (Foster + Freeman VSC 3000) and the spectra were recorded between the light spectrum wavelengths 400 nm to 1000 nm at a resolution of 3 or 4 nm. The visible light spectrum 400–700 nm can be extracted from the data.

For the analysis in FTIR (Nicolet 5700 FTIR-ATR), the scraped bone powder was placed and pressed against the ATR crystal, the infrared spectrum was scanned and converted to absorbance mode. The following working parameters were set: wavenumber range 2000 to 400 cm^{-1}, resolution 4 cm^{-1}, number of scans 16 and automatic baseline correction was performed on the spectra.

Limitations

The current dataset does not offer reference material from experimental cremations. In some instances, the data should be complemented with reference material from experimental cremations in controlled temperature and known heating periods.

The data comes from an archaeological site where bones were fragmented and commingled. Therefore, the determination of the bones based on morphology is limited and the dataset does not offer information on specific bone elements or even body parts.

Some of the spectra are noisy and may not be useable for all purposes. However, since all the samples have been measured twice, so in case of any excess noise, the better-readable spectrum of the same bone can be used.

Ethics Statement

The authors have read and follow the ethical requirements for publication in Data in Brief and confirm that the current work does not involve live human subjects, animal experiments, or any data collected from social media platforms.

Credit Author Statement

Anu Lillak: Conceptualization, Investigation, Writing-Reviewing and Editing, Original draft preparation. **Tim Thompson:** Methodology, Software; Writing-Reviewing and Editing. **Mari Tõrv:** Writing-Reviewing and Editing; Funding acquisition. **Ester Oras:** Writing-Reviewing and Editing; Funding acquisition.

Data Availability

TIR-ATR and VSC measurements on cremated archaeological bone from Aakre Kivivare tarand grave, Estonia (Original data) (Zenodo).

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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