H59 X-ray Diffraction (XRD) Analysis of Human Cremains and Concrete

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The goal of this presentation is to propose a new technology and method for the analysis of human cremains to distinguish between legitimate and contaminated ashes.

This presentation will impact the forensic science community by. The attendee will have increased awareness of x-ray diffraction technology to enhance the scientific analysis of powderized human cremains, which is the standard product of the crematory industry and which typically has no visually recognizable bone fragments.

In the continuing pursuit to objectively characterize human cremains and to identify those that have been substituted or contaminated, we have determined the mineralogy of cremains and Portland cement and a combination thereof using powder x-ray diffraction (XRD). Previous research used inductively-coupled plasma optical emissions spectroscopy (ICP-OES) to sort these same samples based on their chemical composition. The present study has demonstrated that, although chemistry is a good discriminator, the presence or absence of specific crystalline substances, as determined by XRD, may distinguish potentially contaminated cremains that were not iden- tified as such by ICP. This methodology for analysis of cremains had not been proposed in the forensic anthropology literature at the time of the Tri- State Crematory Incident (February 2001, Noble, Georgia).

Powder XRD is used to measure the very small (angstrom-scale) dimensions between atomic planes in crystal structures, which serve to identify and characterize crystalline materials. Sample preparation requires only that the material be ground to a flour-like consistency (1 to 5 µ) and loaded into a sample holder. For the present study, using a Philips diffraction patterns were acquired for 5° to 90° 2\ radiation, and standard procedures PW1830/3550/3710 diffractometer, Cu K and analytical conditions. To identify crystalline substances, diffraction patterns were compared with the ICDD reference database.

Samples used for the present study include the known cremains of 8 adult humans (six white males, two white females) and one *Canis familiaris*, one questionable set of cremains returned from the Tri-State Crematory, one sample of Type I general purpose Portland cement, and one sample of a 50/50 mixture of known human cremains and Portland cement. All 12 samples were submitted to the XRD lab at UTC without any identifying labels, with only the knowledge that the samples include human cremains.

Peaks due to hydroxylapatite (56 peaks in combined reference patterns 24-0033, 09-0432, and 34-0010, 5° to 80° 2\) dominate diffraction patterns for the eight samples of human cremains and that two of *Canis*. Numerous extra peaks (not matched by hydroxylapatite) in these patterns suggest minor abundances of lime, sphalerite, sal ammoniac, sylvite, or other phosphates, but have proven difficult to match with certainty and may reflect chemical and structural complexities of biological hydroxylapatite and its cremation- related alterations. Although the sample from the Tri-State Crematory was found to contain hydroxylapatite (Hap) and was classified as human cremains based on ICP analysis, it was also found in the present study to contain signif- icant amounts of mullite (Mul), kyanite (Kya), and corundum (Cor), common ingredients of refractory furnace linings and patching products. Calcium silicates (Ca3SiO5 and Ca2SiO4) were identified in the sample of Portland cement; the absence of hydroxylapatite in this sample rules out the presence of cremains. Although the 50/50 mixture was not recognized as such in the blind analysis, it was suspected of being contaminated cremains based on the identification of hydroxylapatite and the undue complexity of the diffraction pattern (31 unmatched peaks, some prominent). Upon subsequent examination of diffraction patterns for the 50/50 mixture and its components, their relation is clear. These results are summarized below:

Sample #	Material	XRD Result (Identity)	Unmatched peaks)1(5° to 80° 2
1	human cremains	Hap	12
2	human cremains	Hap	5
3	*Canis* cremains	Hap	27
4	human cremains	Hap	12
5	human cremains	Hap	11
6	human cremains	Hap	12
7	Tri-State cremains	Hap, Mul, Kya, Cor	5
8	human cremains	Hap	16
9	human cremains	Hap	14
10	human cremains	Hap	14
11	Portland cement	Ca3SiO5, Ca2SiO4	6
12	50/50 #6/#11	Hap	31

In conclusion, powder XRD may be sufficient to discriminate cremains from those that are substituted or substantially contaminated. Undoubtedly, the combination of powder XRD, to identify crystalline substances, and ICP, to determine chemical composition, more perfectly authenticates cremains based on more complete compositional criteria. XRD is simpler in laboratory prep time, costs less per sample, and is widely available. These high-tech laboratory instruments, coupled with traditional anthropological methods (weight, color, fragments, artifacts) when applicable, take the analysis of human cremains to an unprecedented level of scientific objectivity.

Human Cremains, X-ray Diffraction, Hydroxylapatite

