Molecular and Structural Archaeology: Cosmetic and Therapeutic Chemicals
NATO Science Series

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PREFACE

Recent progress in the analysis and structural characterisation of materials has an increasing impact on studies of archaeological specimens. A need to embody such research into a new interdisciplinary field has appeared. In this ARW we intended to bring together archaeologists and historians with physicists, chemists, crystallographers and pharmacists, around the theme of structural information on complex archaeological materials. Within this vast area, the ARW has mainly focused on cosmetic-therapeutic chemicals. The objectives of this NATO ARW were twofold:

- Delineating the contour of molecular and structural archaeology as an emerging interdisciplinary field based on structural analysis at the molecular level.

- Examining novel methodologies to reconstruct the scenario of synthesis and transformation in the long term of compounds used in antiquity for health and beauty.

The strong interdisciplinarity of this meeting has been greatly favoured by the NATO ARW organisation allowing the mixing of different fields and disciplines with convergent general goals. This Workshop has shown that the molecular and structural sensibility is a powerful tool towards the setting, and often the solution, of difficult archaeological and historical problems. Ten different nationalities (Europe, Egypt, USA) were represented in the ARW, and this mixing has contributed to the large range of subjects and archaeological contexts. Thus, a mutual interaction between Archaeology and Physical Sciences is expected. The most obvious part is associated with extended use of any possible technique and method to get as much information about the archaeological samples as possible. However, there is its counterpart in the sense that chemistry and physics can learn from samples which are thousands of years old. The long-term transformations of physicochemical systems may be studied in this perspective. It seems we are at the infancy of that approach to the science of ancient materials.

Recent advances in analytical chemistry and crystallography open new perspectives in the study of complex materials and preparations. Many cosmetic-therapeutic materials both inorganic and organic, found in closed vessels in ancient tombs have been completely identified. In this particular study, the molecular and structural information has revealed that the Ancients had developed as early as 2000 BC the technology needed to synthesise these materials, such as wet chemical syntheses of new compounds not known as natural products. This chemical technology was followed by an art of formulation. Nonetheless, the resulting preparations may have been cosmetic or therapeutic, yet their use may also have been associated with ultimately adverse effects on the whole of society, such as long-term lead poisoning.
It is important at this point to enquire about each compound bearing information relating to the time at which it was created and used. The reference to archaeological data and ancient texts is crucial in tracing down this historical information.

Such a shifting from technological and pharmaceutical problems to the history of societies should be the goal of an interdisciplinary debate. The incidence of the recorded physical and chemical data at the molecular level may lead to an important distinction between an *a priori* historical interpretation (i.e. without these data) and an *a posteriori* historical interpretation (i.e. given these data) in a particular archaeological context.

The original objects may also undergo their own materials history at the atomic and molecular level. This consists of alteration or reaction with other compounds, or simply conservation on account of exceptional circumstances. Even if alteration occurs this may not imply total destruction and erasure of all information. The genesis of a new compound may not preclude the retention of significant morphological characteristics of the original one, as illustrated by the beautiful example of mineralised fabrics (slow mineral formation keeping the texture of the initial biological material). Modern methods are able to analyse the supramolecular organisation of materials as complex as wool, hair or skin. Here, we have to take into account the archaeological periods of time as a "fourth dimension in chemistry" measured in centuries and millennia, in order to approach the significance of the "molecular messenger" as found at the present time. Many difficult problems arise from the complex alteration of the initial materials - and sometimes from a surprising stability, for instance, in the conservation of structurally organised unsaturated fatty acids. One could stress the difficulty of designing a type of simulation experiments to shed light on the long term alterations. Such new problems emerging in the course of analysis and structural characterisation may often be at the frontier of the today's technologies and even at the edge of current scientific concepts. It is then indispensable to undertake fundamental research that would push further the limits of the available methods. Moreover, the complexity of many materials is such that a single technique is not sufficient: discussion of upgrading and combining novel methodologies will be an objective of this ARW, including Crystallography, Synchrotron Radiation Techniques, Raman and Infrared Microscopy and Cartography, Analytical Chemistry, and others. One should stress the role of non-destructive methods in the identification of archaeological objects.

Clearly, such research work relies strongly upon structural information at the molecular and supramolecular level. In particular, simulation experiments for long-term transformations involving an artificially accelerated ageing process carried on in the laboratory should be based on a precise knowledge of the structural, physical and chemical phenomena occurring at the molecular and atomic scale. For instance: oxido-reduction phenomena; diffusion of metal ions into specific sites in wool, hair and skin; loss of crystallinity, or, on the contrary, long-term
crystallisation, or more generally variation of the degree of order and supramolecular organisation; crystalline imperfections consecutive to carving, grinding, crushing and annealing (revealed by microstructural characterisation). Thus, the nature of the initial materials and the techniques necessary to their preparation by the Ancients may become accessible, and ultimately related to an archaeological context and to the History of Societies. Hence we feel the need for a dialogue between physicists and chemists with archaeologists and historians. Furthermore, recording and discussing progress in these areas will contribute to new advances in Conservation Science.

Similar advances have recently been recorded in other areas involving “molecular messengers”. In the proposed ARW we endeavour to delineate a contour of Molecular and Structural Archaeology where future meetings could focus on DNA and other biological investigations, food remnants, binders, varnishes, pigments, and others.

Four themes have been highlighted in the present ARW:

1. Reconstruction of a scenario of synthesis and production of substances for health and beauty

2. Methodology for physical and chemical analyses

3. Long run transformation of ancient materials as a “fourth dimension” in molecular and supramolecular chemistry.; simulation experiments

4. Delineating a contour of Molecular and Structural Archaeology as an emerging interdisciplinary field based on structural analysis at the atomic level.

The present Advanced Research Workshop ARW is the first activity of a new School “Molecular and Structural Archaeology” created at the Ettore Majorana Centre and directed by Professor Hubert CURIEN, president of the Académie des Sciences.

The ARW was run in parallel with the 33rd Course of the Crystallography School. The organisation of the ARW has been greatly facilitated by the support of Dr Nera BORKAKOTI, director of the Crystallography Course, and Professor Sir Tom BLUNDELL, director of the Crystallography School, as well as by the experience and skills of Professors Lodovico RIVA DI SANSEVERINO and Paola SPADON.

Georges Tsoucaris
Janusz Lipkowski