

INFLUENCE OF MORDANTS IN THE COLOUR OF NATURAL DYES: THEORETICAL PREDICTIONS AND EXPERIMENTAL RESULTS

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Abstract

Arraiolos tapestries are probably one of the richest artistic Portuguese expressions in terms of textile production and a cultural heritage that urges to preserve. The richness of colours displayed by some of the Arraiolos tapestries denotes the likely use of a wide variety of dyes. The different light-fastness of dyes combined with the use of different types of mordants can also explain the appearance of pale shades and fading in some tapestries due to different molecule interactions with the support fibres.

The work we present is part of a major project (experimental and theoretical) that envisages the identification of the dyes and mordants used throughout the ages in the production of Arraiolos tapestries and the establishment of the major factors (like mordant, humidity and light) that are responsible for the colour and fading of the natural dyes as well as for the degradation of the fibres.

It is well known that the colour of a dye depends on the type of mordant used, due to the formation of metal complexes that cause a change in the molecular orbitals energies and hence a shift in UV/Vis absorption bands.

The electronic structure and transitions in the visible spectra of some dyes and mordants identified on Arraiolos rugs were predicted by the ZINDO-INDO/S semi-empirical molecular orbital method [1,2] in order to identify the origin of the colours and characterize the influence of metal coordination on colour modifications. The molecular geometry of each dye-mordant complex was optimized at DFT level using the Gaussian03 package [3] and a simulation of the UV/Vis absorption spectrum was calculated using ZINDO.

Another important outcome of this study was the determination of the chromophore properties of fragment molecules produced by the dyes degradation processes that enabled the evaluation of the colour changes of the dyes and subsequent fading.

Wool fibres were dyed with previously identified natural dyes and mordants and the colour parameters and the spectra were determined using a UV-Vis portable spectrometer. These parameters were compared with the results from the theoretical predictions.

References

- [1] Ridley, J.; Zerner, M. *Theor Chim Acta* 1973, 32, 111–34.
- [2] Zerner, M.C.; Loew, G.H.; Kirchner, R.F.; Mueller-Westerhoff, U.T. *J Am Chem Soc* 1980, 102, 589–99.
- [3] Gaussian 03, Revision C.02, Frisch, M. J. *et al.*; Gaussian, Inc., Wallingford CT, 2004.