THE USE OF LINEAR FREE ENERGY RELATIONSHIPS IN THE INVESTIGATION OF A ZIRCONIUM COMPLEX TANNING AGENT

J. J. Guthrie-Strachan[1], E. M. Antunes[2], A. P. M. Antunes[1] and G. M. Watkins[2]

[1]British School of Leather Technology, The University of Northampton, Boughton Green Rd, Northampton, NN2 7AL, United Kingdom
[2]Rhodes University, P. O. Box 94, Grahamstown, 6140, South Africa

Abstract: In an effort to better evaluate the nature of the Zr-O bond, several zirconium α-hydroxycarboxylate complexes with various *para* derivatives of mandelic acid were examined to identify any structural activity relationships that may exist. This may assist understanding the potential role of zirconium α-hydroxycarboxylates as tannages in terms of possible binding to collagen, and the stability of the metal complex.
Principles underlying reactivity and free energy relations of a multitude of heterolytic reactions of substituted benzene reactions can be ascribed by the classical Hammett equation defining the structural activity relationship for the rate of hydrolysis of benzoic acid derivatives. Hammett σ plots and Yukawa-Tsuno modified σ plots of the mandelate ligand and zirconium complex series indicated that inductive effects dominate within the benzene ring, however, mesomeric effects are significant outside the ring.