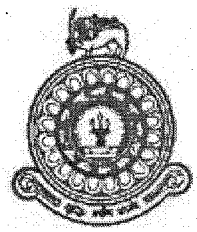
Development of a low cost method for the speciation of chromium in water

By

Experimental and Computational model



Dissertation submitted in partial fulfillment of the requirements of the degree of **MASTER OF SCIENCE IN ANALYTICAL CHEMISTRY**

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Abstract

A low cost experimental procedure for the determination of Cr (VI) and Cr (III) and a computer model based on aqueous phase equilibria of different chromium species were developed. The experimental procedure involves the quantitative generation of iodine by Cr (VI), solvent extraction of such generated iodine into dichloromethane and subsequent determination by UV- visible spectroscopy. High colour intensity and extraction efficiency of iodine makes it possible to detect chromium concentrations as low as 0.07± 0.07μg cm^{-3}.The absorbance of iodine extraction into the organic layer is linearly correlated with the concentration of Cr (VI) in the aqueous layer and the correlation coefficient was found to be around 0.97. The effect of Cr (III) on the determination of Cr (VI) was studied in detail. Further, the effects of electrolytes concentrations, temperature and the time required for the completion of iodine generating reaction were investigated. The method gave the best sensitivity in the temperature range of 40 ^{0}C – 50 ^{0} C. The electrolyte concentration did not show a significant effect and the presence of Cr (III) showed slight enhancement of Cr (VI) detection. It is speculated that this is due to the conversion of a small fraction of Cr (III) into Cr (VI). The optimum time for the completion of reaction was found to be 15 minutes. Longer times than that causes the evaporation of iodine from the aqueous layer at higher concentrations. Total chromium is detected by atomic absorption spectroscopy. Then Cr (III) concentration could be determined by using the Cr (VI) concentration determined by the method developed and the total chromium concentration.

The computational model facilitates the analysis of experimental results. It predicts the concentration of all species of chromium at given total chromium, pH and pE (inverse log of electron activity).The validity of the model is checked out using literature cited experimental data.