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The work described in this thesis was carried out by me under the supervision of Dr. P.M. Jayaweera and a report on this has not been submitted to any University for another degree.

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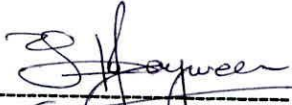
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**SPECTROSCOPIC AND ELECTROCHEMICAL STUDIES
OF IRON(II) AND COBALT(II) COMPLEXES;
POTENTIAL DYE MATERIALS FOR NANO-POROUS
PHOTOVOLTAIC DEVICES**

By

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Philosophy in Chemistry of the Faculty of Applied Science, University of Sri
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ABSTRACT

Metallochromic triphenylmethane type dyes (bromopyrogallol red and catechol violet) have attracted attention of many scientists due to their potential ability to chelate with a number of transition metal centers. The dye materials belonging to this class is capable of producing high photocurrents and photovoltages when used as sensitizers in nano-porous TiO₂ photovoltaic cells. However, slow photo-degradation of dye molecules and low photocurrent conversion efficiencies have been the major problem.

Complexation of a triphenylmethane ligand with a transition metal center shows enhanced photovoltaic properties when compared with the photovoltaic cells coated by free triphenylmethane ligand only. Electrochemical and absorption spectroscopic data suggest that the nature of the lowest electronic transition of such a complex as a π^* (ligand) $\leftarrow d \pi$ (metal), metal to ligand charge transfer transition. Photovoltaic cells coated with these transition metal complexes show higher stability for photo-degradation and incident photocurrent conversion efficiencies with a UV radiation blocking filter.

When catechol violet is complexed with Co²⁺(1,10-phen)₂ moiety, it shows emission as well. Experimental and theoretical data suggest that the emission of this complex occurs from an upper ligand centered state and not from a low lying MLCT state.

1,2-dihydroxyanthraquinone or 1,2,5,8-tetrahydroxyanthraquinone can be used as sensitizing dye material in nano-porous solar cells, not only they produce fairly high photocurrent and photovoltage, when exposed to light, but also those properties show high sensitivity to the protonation and deprotonation of the 2 hydroxy group of the ligand when the pH value of the solvent is changed. Semi-empirical computational studies have shown that fine tuning of HOMO-LUMO orbitals are responsible for the sensitivity.