# "THEORETICAL INVESTIGATIONS ON MOLECULES"

*by*

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*A thesis submitted for the Degree of Master of Philosophy at the University of Colombo, Sri Lanka.*

OCTOBER 1980.

## SUMMARY

The research presented in this thesis can be broadly classified into four categories.

The first category involves Semi-Empirical Molecular Orbital Calculations on pi electron systems. A Semi-Empirical Molecular Orbital method for pi systems is developed and used to study molecular properties like ionisation potential, electronic spectra, charge density, bond order distributions and gradation of the aromatic stabilisation of conjugated systems.

The next section involves extension of the method to larger systems. This is done by considering the large system to be 'constructed' from smaller constituent systems of comparable geomerty, referred to as 'framework' molecules, for which calculations using the method described earlier have been carried out. The problems studied using such a technique are the anti-bacterial activity of acridines, the toxicity of Nitrophenols towards bacteria and the regioselectivity in the Diels-Alder reaction.

Sigma electron systems are next treated by two methods: (a) A modified Complete Neglect of Differential Overlap (CNDO) scheme; and (b) ab-initio methods. The CNDO method is modified and applied in studying molecular properties of some simple diatomics. The ab-initio method involves the use of correlated gaussian functions to enhance the convergence of the Configuration Interaction (CI) wave function. The investigations are preliminary and were carried out on the Hydrogen molecule.

Finally, a qualitative approach based on substituent and solubility factors is discussed in the rationalisation of the Carcinogenic nature of Aromatic Amines.