CHAPTER 9: SUMMARY

The structure of m-toluic acid and the stereo-chemistry of RuCl$_2$(CC)$_2$(Ph$_2$ Et As)$_2$ have been determined.

The structural analysis of m-toluic acid (3-methyl benzoic acid) was undertaken to study the influence on the molecule structure of a methyl group substituted in the meta position in benzoic acid. The compound crystallizes in the space group $P 2_1/C$ with two molecules in the asymmetric unit. The Patterson synthesis showed a benzene ring at the origin. Attempts were made to solve the structure of Patterson methods, these did not yield successful results. The structure was finally solved by direct methods. The symbolic addition method was used to solve the phase problem. For this purpose, Fortran programmes of Hall and Ahmed were modified for use on an IBM 360/44 computer. The following programmes were written and used for structural work.

i) Data preparation

ii) $L_2$ factor and absorption corrections

iii) $P 2_1/C$ Fourier (3 dimensional)

iv) $P 2/m$ Patterson with sharpening (3 dimensional)

v) $P \bar{1}$ Fourier and Patterson (zero layer)
Unlike the majority of carboxylic acids, m-toluic acid does not form dimers about a crystallographic centre of symmetry. Dimers are formed at general positions between the two crystallographically non-equivalent molecules. There is a planar stacking of molecules (separation distance of 3.57 A.U.) with an inter-molecular contact of 3.28 A.U. between the two carboxyl groups. Another short intermolecular contact of 3.34 A.U. exists between a methyl carbon and an oxygen atom of an adjacent molecule. The configuration adopted involves:

a) Hydrogen bonding in the dimer
b) Formation of a very weak self complex between the molecules which are parallel
c) Formation of weak bonds of the type $C=O...C$, $CH_2...O$.

The structural analysis of a ruthenium complex, dichlorodicarbonyl bis diphenyl ethyl arsene ruthenium II - was undertaken to investigate the stereochemistry of the molecule. This compound crystallizes in $P1$ or $P1\bar{1}$, and has two molecules in the unit cell. The $a$ and $c$ axes projections have been studied and the heavy atoms ruthenium, chlorine and arsenic have been located.

Of the five possible configurations, the infrared and
NMR spectra showed that the following were possible.

The X-ray studies indicate that the configuration I is adopted.