CHAPTER 1

INTRODUCTION

Triniobium arsenide(Nb_3As) was prepared by melting mixtures of niobium and niobium arsenide(NbAs) under purified argon, and the system perhaps consisted of four intermediate phases, Nb_3As, Nb_7As_4, Nb_5As_3 and $NbAs_{\sim 0.75}$(Rundqvist, Carlsson and Pontchour, 1969). Nb_3As appears to be the most metal-rich compound in the system.

In this work, the structure of triniobium arsenide has been determined and refined by X-ray diffraction analysis. It is found to be isotypic with the structure of Nb_3P which was previously determined by Nawapong et al (1966).

Some details of the work involved are to be reported in the four remaining chapters.

The diffraction process essential to the application of X-ray methods to structural problems is introduced in chapter two , and the general steps in a crystal structure analysis are shown in the last part of the chapter.

Chapter three describes how a single crystal is chosen and mounted, and how the cell constants and the space group of the sample can be determined from the pattern of the X-ray diffraction by the crystal on various kinds of X-ray diffraction photographs. Finally, the collection of the intensity

data is described.

Chapter four deals with the calculation of the location of all atoms in the unit cell from the collected intensity data. These atomic positions are refined by Booth's method and finally by the least-squares method. The final co-ordinates of all atoms, their thermal parameters, bond lengths and angles are given.

Chapter five includes conclusions and discussions of the final results.