

**STUDIES ON STATISTICAL INFERENCE FROM X-RAY
AND OTHER SPECTROSCOPIC DATA**

By

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**A THESIS
SUBMITTED IN FULFILMENT OF THE
REQUIREMENT FOR THE DEGREE OF
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To



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**“The fear of the Lord is the instruction of wisdom ;
and before honour is humility”**

(Proverb 15 : 33)

*DEDICATED TO
MY PARENTS*

Whose guidance had been the source of this goal.

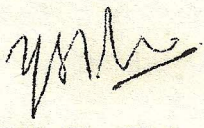
CERTIFICATE

I certify that the dissertation entitled "STUDIES ON STATISTICAL INFERENCE FROM X-RAY AND OTHER SPECTROSCOPIC DATA" submitted by Miss Phlisdamon Nonokynrih in fulfilment of the requirements for the degree of DOCTOR OF PHILOSOPHY is the outcome of a study undertaken by the candidate.

I certify that the sources from which ideas have been borrowed have been duly referred to and acknowledged.

The material in this dissertation has not been presented for award of a degree in any University before. This dissertation may be placed before the examiners for evaluation and necessary formalities.

The work for this thesis is a continuation of the candidate's M.Phil. dissertation entitled "Nuclear Techniques in Trace Element Analysis". The identification of Titanium and the observations on the Crystal Structure changes are worthy of consideration by the examiners for the award of the degree of Doctor of Philosophy.


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P. Nongkynrih.
(P. Nongkynrih)
7th Dec. '85.

(v)

<u>CONTENTS</u>	<u>PAGE</u>
CERTIFICATE	(i)
ACKNOWLEDGEMENTS	(ii)-(iv)
TABLE OF CONTENTS	(v)
CHAPTER 0: INTRODUCTION	1-4
CHAPTER 1: TRACE ELEMENT DISTRIBUTION IN COAL FIELDS OF NORTH-EASTERN INDIA	5-24
CHAPTER 2: STUDYING OF THE RESULTS OBTAINED FROM THE XRF ANALYSIS	25-42
CHAPTER 3: ANALYSIS OF THE X-RAY DIFFRACTION DATA OF THE SUBSTITUTED APATITES	43-74
CHAPTER 4: ANALYSIS OF THE I.R. SPECTRA OF THE SUBSTITUTED APATITES	75-93
CHAPTER 5: CONCLUSION	94-96
APPENDIX A: MEGHALAYA COMES ON THE BAUXITE MAP OF INDIA	97
APPENDIX B: PETROLOGY OF THE CARBONATITES AND ASSOCIATED ROCKS OF SUNG VALLEY, JAINTIA HILLS DISTRICT, MEGHALAYA, INDIA	98-105
APPENDIX C: PREPARATION AND CHARACTERIZATION OF SOLID SOLUTIONS OF PHOSPHATE AND VANADATE APATITES OF LEAD	106-109
APPENDIX D: PREPARATION AND CHARACTERIZATION OF SOLID SOLUTIONS OF PHOSPHATE AND VANADATE APATITES OF CALCIUM	110-112

CHAPTER- 0INTRODUCTION

Physics is a branch of Science which is involved mostly with experiments. One performs the experiments, thoroughly takes the measurement and checks its reproducibility. The data obtained are analysed and consequently the theory often follows to explain and give a proper understanding of the experimental results. In any experimental study, the understanding of the system we study depends upon the precision and reliability of the measurements. In most cases, a systematic logical theory is proposed to give a picture of the phenomena which have not yet found by experiments. This systematic understanding of the physical process becomes a law. If the errors have been taken care of and also if all sorts of precautions are adopted yet if found that the experimental findings differ from the prediction of the law by many times the estimated error, then the law needs modification.

Physics deals mostly with quantitative measurements of physical properties of objects and precise relation between these properties. Hence, Mathematics plays a very important role in Physics.

As our resources are limited and that there could be some factors influencing our measurements which have not been taken into account, the theory of Errors, Analysis of Variance, Design of Experiments, Estimations or in general the science called Statistics is to be used. "By Statistics, we mean aggregates of facts affected to a marked extent by multiplicity of causes, numerically expressed, enumerated according to reasonable standards of accuracy, collected in a systematic manner for predetermined purpose and placed in relation to each other" as defined by Horace Secrist.

The philosophy of Statistical techniques is not well appreciated in our Sister Disciplines and more so in interdisciplinary research. In this thesis, two problems of interest to our friends in sister disciplines- Geology and Chemistry are analysed to demonstrate what they have lost sight of and then the new results brought by the diverse physical (experimental) techniques will be discussed.

The first chapter deals with the X-Ray Fluorescence Technique (XRF) used for detecting and estimating the trace elements in samples. This technique is developed in the last few years and has become an important tool to the geologists, environmentalists, health scientists, etc.

The use of the XRF technique in analysing the trace elements in the coal fields of North-Eastern Region of India is described in the second chapter. The region has got a good reserve of coal. Coal was chosen as it is a repository of elements that are likely to be present in the neighbourhood. The analysis of coal can therefore serve as a precursor in identifying possible location of mineral wealth in the region. Further such analysis may have a bearing on geochronological studies.

The unusual finding of large quantity of Titanium in Bapung (Jaintia Hills District, Meghalaya) which all the previous workers using chemical technique have missed is an important contribution. Following our work, the Geological Survey of India has identified a rich source of Titanium in Sung Valley (Jaintia Hills District, Meghalaya) close to the fields where our study was carried out.

The third chapter deals with the studies involving the analysis of the X-Ray diffraction data of the substituted apatites. Apatites are important constituents of human bone and teeth. Their decay is due to isomorphic substitution of the constituents which affect the changes in crystal structure. The lattice of the apatites is in general hexagonal in structure. According to Vegard's Law the lattice

constants 'a' and 'c' of hexagonal lattice are expected to change linearly with the degree of substitution. So far, it appears that all experimental evidence support this law, we show that the law is violated and that two distinct and different linear behaviors in the ranges 0 - 50% and 50 - 100% degree of substitution are obtained.

The fourth chapter deals with the use of Infra Red absorption spectroscopy technique for the substituted apatites. The results confirm our conclusion that something happens around 50% degree of substitution.

The fifth and last chapter summarise the work described in the previous chapters. It also emphasizes the importance of using statistical and physical techniques in analysing results of important to sister disciplines.