Preface

Coal is one of the naturally available fossil fuels having immense contribution towards energy and power. It is generally made up of heterogeneous materials and its composition varies with the places of occurrences. Its structure, also, changes with its matrix. The use of coal as an energy source and as a source of organic chemicals feedback may become more important in the future. It has a physical micro structure that is discernibly derived from plant and a chemical structure containing a wide variety of polymeric organic compounds and crystalline minerals. Detailed structural characterization has been found to be extremely difficult and therefore, research on coal structure is still a challenging task and continuing to be pursued intensively. Because of the relationship of coal structure to its reactivity in various coal processing and utilization techniques such as combustion, pyrolysis, liquefaction and gasification processes, the structural properties of coal have been receiving much attention among the coal researchers and thus, a deeper understanding of its chemical composition and structural characteristics could result in substantial improvement in coal processing and utilization. The role of X-ray diffraction study in coal science is enormous. It can provide information about the structure of the molecular core of coal. X-ray diffraction data for coal and coal-derived solids are more appropriately considered in terms of their trends and can provide valuable information about structural variations. FT-IR is currently one of the most powerful and versatile technique for the characterization of coal structure. It has several advantages including relatively low instrumental cost as well as fast and easy operation. The structural parameters in coal provide useful information to determine coal rank, utilization and oil
generation capacity. Extraction of coal by solvents has been used for many years for studying the constitution of coal and for producing products of potential industrial value. Microwave assisted solvent extraction has received increasing attention as a potential alternative to traditional solid-liquid extraction methods, mainly due to considerable saving in processing time and solvent consumption.

The structural models is very much useful from both pure and applied research point of view and have been utilized with great success to investigate the mechanisms of the pyrolysis, hydrogenation and hydrocracking reactions including the formation of the products and their control by experimental conditions and catalysis. Progress of knowledge about the chemical structure of coal has opened the door for the simulation of reaction paths by computer modeling. Thus, the study is to be conducted to meet a growing need of systematic databases on structural features of coals from North-East India. This type of databases will be valuable in the application of these coals for technological utilization.

The present investigation is concerned with the structural study of coal from North-East region of Makum collieries, Assam, India particularly Tirap colliery from various depths using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR) and physico-chemical analysis. The XRD method includes the evaluation of function of radial distribution of atoms (FRDA) of coal, to determine the short-range structural features of coal, to describe the details of the average polycyclic aromatic unit in coal and structural interpretation of the coals from their radial distribution function (RDF). The evaluation of carbon stacking layered structure of the coals from their X-ray diffraction patterns were done in this study. The X-ray structural parameters for carbon random layer
structure includes the evaluation of the carbon stacking layered structure of coal, the average stacking height of the parallel aromatic layers in the c-axis direction, the average diameter of the parallel aromatic layers, the total numbers of layers, the total number of carbon atoms present per layer etc. The estimation of the aryl and alkyl fraction in the coal from its RDF analysis is, also, included in this study. Fourier Transform Infrared Spectroscopy was included for assignment of different functional groups present in the coal structure. In this work quantitative structural study particularly oxygenated functional group and characterization of oxygenated functional group, the structural parameters from FT-IR spectra which includes the fraction of aromatic and aliphatic hydrogen contents, fraction of aromatic and aliphatic carbon content and the fraction of aromatic carbon, i.e. aromaticity (fa) of North East India coal have been carried out using the FT-IR spectroscopic technique. Difference FT-IR spectroscopy was used to study the structural components of coal extracted with the help of microwave assisted solvent extraction procedure in two different solvents ethyl acetate and carbon tetrachloride. A systematic physico-chemical analysis of coal samples was, also, performed to have better knowledge on structural aspects of the coals from this region. These analyses include proximate analysis, ultimate analysis and fraction of hydrogen to carbon and oxygen to carbon ratio of the North-East India coal.

A comparative study on structural properties of the coal samples of different depths from Tirap colliery of Makum coalfield from North-East India was discussed in this study. The results obtained in this investigation will be helpful in gaining an insight in to the
structure of these coals for better understanding the potential problem for their industrial utilization.

The thesis consists of five chapters as described below,

**CHAPTER I: INTRODUCTION**

This chapter describes the general introduction of the subject with origin and formation, classification and structure of coal. This chapter gives some information on the past and present status of the research activity in this subject along with the main objectives of the present works.

**CHAPTER II: METHOD AND THEORY FOR STRUCTURAL INVESTIGATION OF COAL**

This chapter describes the theory and method for studies of North-East India coals by Function of Radial Distribution Analysis (FRDA) using X-ray diffraction data. The methodology of Fourier Transformation Infrared Spectroscopy (FT-IR) is, also, included in this chapter. The chapter, also, includes chemical analysis of the coal samples.

**CHAPTER III: STRUCTURAL MODEL OF COAL FROM TIRAP COLLIERY FROM MAKUM COALFIELD, ASSAM, INDIA (20ft seam)**

This chapter is related with the structural investigation of coal sample from Tirap colliery of Makum coalfield, Assam, India of 20 ft seam at a depth of 100 m from the surface. X-ray diffraction, FT-IR and other analytical techniques were used to study the structural model of the aromatic micro-domain of the coal samples.
CHAPTER IV: STRUCTURAL MODEL OF COAL FROM TIRAP COLLIERY FROM MAKUM COALFIELD, ASSAM, INDIA (60ft seam)

This chapter is related with the structural investigation of another coal sample from Tirap colliery of Makum coalfield, Assam, India of 60 ft seam at a depth of 150 m from the surface to investigate the variation in structural properties with depth. Thus, this chapter mainly deals with the study of structural model of the aromatic micro-domain of the coal sample by the X-ray diffraction, FT-IR and other analytical techniques.

CHAPTER V: A COMPARATIVE STRUCTURAL INVESTIGATION OF NORTH-EAST INDIA COALS

As the structural features of coal changes with depth, this chapter describes the structural investigation of molecular level structure of Tirap coal of different depths. This investigation includes Function of Radial Distribution of Atom (FRDA), Fourier Transform Infrared Spectroscopy (FT-IR) structural analysis and physico-chemical characterizations of coals.