Thiourea and its derivatives have found their way into every branch of science. They possess a variety of pharmacological, agrochemical and industrial applications. In pharmaceuticals they are used as anti-tubercular, anti-thyroidal, anti-bacterial, anti-viral, anti-depressant and anthelmintic agents. A lot of thiourea derivatives have insecticidal, anti-viral, fungicidal, and herbicidal properties. Thiourea and its derivatives are suggested as good corrosion inhibitors for metals and alloys.

The biological and chemical properties of thiourea derivatives depend on its structure, especially the configuration of the substituted groups and the hydrogen bonding ability. Although structure activity relationships have been established earlier, there is no structural report exclusively concerning substituted thiourea derivatives available. Only crystal structure analyses of metal complexes of thiourea and a few substituted thioureas have been reported. This may be due to the difficulties encountered in obtaining crystals suitable for X-ray diffraction studies, but in our laboratory sixteen thiourea derivatives were successfully crystallized. Of the sixteen compounds, seven are symmetrical and the remaining nine are unsymmetrical thiourea derivatives. These derivatives have applications in pharmacology and chemical industry.

The X-ray crystal and molecular structure determination of these compounds were taken up in a view to study the molecular conformations, N-H...S hydrogen bond formation and packing details in the solid state.
Since the major part of the thesis deals with crystal structure analyses, Chapter 2 gives a brief introduction of crystal structure determination. The details of X-ray crystal structure determination of these compounds are given in Chapter 3 to Chapter 10. Some of these compounds were tested for their antibacterial and anticorrosion behaviour and the results are given in Chapters 11 and 12. Chapter 13 contains the conclusion of these studies. Crystal structure analyses of the substituted thiourea derivatives reveal that they can exist in either trans-cis or cis-cis configurations. Even though cis-cis configurations are energetically favoured, trans-cis is observed predominately in the solid state.

The trans-cis configuration allows the molecules to form dimers through N-H...S hydrogen bonds. The dimers are either centrosymmetrically related or 2-fold related. Only one of the two NH groups (N1) is engaged in the dimer formation. N2 takes part in the H bond schemes only in certain arrangements or situations and it depends on the substituents. In general, N-H...S bonds involving N2 is weaker than the N1-H...S. N2-H...S connects the dimers and leads to the formation of two dimensional nets of molecules in certain cases. If the dimers are formed between 2-fold related molecules, N2 does not take part in any H bond scheme. In cis-cis configuration, there is no room for the dimer formation and the molecules can only form chains through three centre N-H...S bonds. Among the symmetrically substituted thiourea derivatives, only 1,3-diphenylthiourea has the cis-cis form and 1-cyclohexyl-3-(2-tolyl)thiourea of the unsymmetrical thioureas exists in the cis-cis configuration.
The major differences found in the geometrical parameters of these thioureas are the C1=S distance and the bond angles around C1. In DPTU, DEPTU and OCDPTU structures the C=S is equal to the reported values in literature and in the rest of the structures C=S is longer. The N1-C1-N2 angles are wider in trans-cis forms than in the cis-cis compounds and the corresponding effects are observed in N1-C1-S and N2-C1-S angles. In these derivatives, the N-C(ar) distances are longer than the mean value 1.353Å reported in the literature.

Anti-bacterial effects of some thiourea compounds were assayed by the Broth dilution technique. The bacterial cultures used were: 1. Staphylococcus aureus (SA), 2. Proteus mirabilis (PM), 3. Pseudomonas Aeruginosa (PA), 4. Escherichia coli (EC), 5. Salmonella typhi (ST), 6. Shigella flexneri (SF), 7. Vibrio cholera (VC) and 8. Klebsiella pneumoniae (KP). The compound DEPTU inhibited all eight bacteriae, DPTU inhibited SA, EC and KP, DETU inhibited PA, ST, VC and KP, CHTTU inhibited ST and KP and ALPTU inhibited PM and EC.

Anti-corrosion behaviour of some of the thiourea derivatives were performed with a mild steel specimen in HCl. The thiourea derivatives are found to be better corrosion inhibitors for mild steel in acidic solutions than the thiourea alone. The enhanced inhibitory action exerted by these derivatives can be attributed to the substituents present in the thiourea molecule. These substituents influence the inhibitory action of molecules by decreasing the solubility and increasing the chemisorption through the delocalized electron clouds around the phenyl ring besides providing better surface coverage.