ABSTRACT

The main subject matter of this work is the determination of molecular and crystal structure of amobenzene-2-sulphenyl cyanide. In investigating the trial structure free use of the optical transform technique has been made at the initial stages. The structure has, however, been refined by two-dimensional Fourier synthesis. In chapter one, the general principles of the application of optical-transform methods have been described, along with a short description of the "Optical diffractometer".

The second chapter has been devoted to discuss in brief the chemistry of amobenzene-2-sulphenyl cyanide. Determination of unit-cell and space group has also been discussed here.

In the third chapter, the procedures adopted for obtaining the approximate structure have been described. The derivation of unitary structure factors, the scope of optically derived transform, and the importance of the weighted reciprocal lattice in providing informations regarding significant structural features have been dealt with. Further, the use of Patterson synthesis to locate the sulphur atom of the amobenzene-2-sulphenyl cyanide molecule has been discussed in this
The refinement of the trial structure of the centrosymmetrical c-axis projection has been discussed in chapter four. In the earlier stages of refinement of procedure of optical sign determination has been used for obtaining the signs of the structure factors.

Refinement of the (001) projection by \((P_0 - P_g)\) synthesis has been discussed in chapter five. An attempt to locate the hydrogen atoms from the \((P_0 - P_g)\) synthesis and the use of optically derived transform to locate the same have been discussed here. The difference Fourier map has been exploited to the extent of adjusting the individual temperature factor parameters of some of the atoms including the anisotropic temperature factor parameter of sulphur. Extinction correction for some of the low-angle strong reflexions and use of these corrected structure factors in re-drawing the electron-density map has been included in the same chapter.

The sixth chapter has been solely devoted to discuss the work along the a-axis projection. Refinement of the \(z\) parameters by Fourier and difference
Fourier synthesis has been dealt with.

The final atomic co-ordinates, bond-lengths, bond angles and intermolecular approaches have been given in the last chapter. Geometry of the azobenzene-2-sulphenyl cyanide molecule, statistical assessment of accuracy in the evaluation of electron-densities and atomic co-ordinates have been done in this chapter.