SYNOPSIS

This thesis embodies the details of crystal structure analyses of two compounds, bis (pyrazine - 2:3 - dicarboxamide) copper (II) perchlorate and (-19, 20* cyclopodocarpa - 19 - oxo - 8,11,13 - triene. Answers to two different questions were sought for in the two investigations. For the first compound the problem was to find the nature of coordination of the copper atom; the second compound presented the problem of determining the conformation of the bridge ketone molecule. Solutions of both these problems called for determination of the crystal structures by X-ray diffraction techniques.

Chapter I of the thesis starts with the specification of the scope of the thesis. This is followed by a brief outline of the method of crystal structure analysis. The procedure actually used in the present investigation has been narrated step by step.

Determination of the crystal structure of bis (pyrazine - 2:3 - dicarboxamide) copper (II) perchlorate has been described in chapter II. The crystals are triclinic, with a = 12.21(8), b = 7.65(6), c = 11.06(8) Å, α = 84.75°(4), β = 101.5°(5), and γ = 96.9°(5); the space group is Cī, with Z = 2. The C - centred cell has been used because this particular choice of axes proved to be very convenient in describing the nature of twinning prevalent in these crystals. Almost all the crystals were found to be twins, with two components related by a two-fold rotation about the b-axis common to both the components.

The structure was solved by three dimensional Patterson synthesis. A full-matrix anisotropic refinement of 953 photographic data yielded a final R - value of 0.09. The results obtained reveal a square - planar coordination of Cu with one carboxamide O and one pyrazine N from each of a pair of centro symmetrically related ligands. There is no participation of any perchlorate oxygen in the coordination. The prevalence of twinning giving rise to a monoclinic pseudo - symmetry suggests a probable existence of a monoclinic phase at some higher temperature.
In Chapter III, the determination of the crystal and molecular structure of the bridged tetracyclic ketone (±) - 19, 20 - cyclopodocarpa - 19 - oxo - 8,11,13 - triene has been described. The crystals are monoclinic, space group P2₁/c, with a = 8.41(2)Å, b = 7.40(2)Å, c = 21.04(6)Å, β = 94.0(4)° and Z = 4. The structure was solved by direct method from visually estimated photographic data, and was refined by full - matrix least squares method to an R value of 0.109 for 985 observed reflections.

The results show that the A ring assumes a distorted chair configuration while the B ring, adjacent to the aromatic ring, takes up a distorted boat configuration. The ring current of the aromatic moiety seems to have percolated to the adjacent parts.