

# Crystal Structure of Diphenyl Pyraline Hydrochloride—Cobalt Chloride Complex

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The crystal structure of the complex of diphenyl pyraline hydrochloride with cobalt chloride,  $C_{38}H_{46}O_2N_2Cl_4Co$  has been determined by X-ray diffraction using  $CuK\alpha$  radiation. The compound crystallizes in monoclinic space group  $P2_1/n$  with the cell parameters  $a = 18.120(4)\text{\AA}$ ,  $b = 8.179(3)\text{\AA}$ ,  $c = 26.805(3)\text{\AA}$ ,  $\beta = 102.60(1)^\circ$  with  $Z = 4$ ,  $V = 3876(1)\text{\AA}^3$ . The structure was solved using 5484 reflections. The structure was refined to a final  $wR$  of 0.2944 ( $R = 0.1130$ ). The packing of the molecules shows a layered arrangement.

*Keywords: Crystal structure, diphenyl pyraline hydrochloride, cobalt chloride*

## INTRODUCTION

In this paper, we report the results of the structural analysis of a complex of an antihistamine drug, diphenyl pyraline hydrochloride (DPH). The chemical name of DPH is 4-diphenylmethoxy-1-methyl-piperidine hydrochloride. It has found extensive use as a medical agent<sup>1–7</sup> and as an antioxidant in industry.<sup>8–9</sup> Its fungicidal activity has been studied.<sup>10,11</sup> The crystal structure of DPH is reported earlier.<sup>12</sup> In this paper the crystal structure of the complex of cobalt chloride with DPH is reported. The complexes of Co(II) with DPH are found to have increased fungicidal activity beyond a certain concentration level.<sup>13</sup> The fungicidal activity of these complexes were checked on *A alternaria alternata*, a fungus isolated from sunflower plants.

## EXPERIMENTAL

The complex was synthesized by mixing hot ethanolic solutions of Co(II) salt with DPH in 1:2 stoichiometry. The solid formed under slow evaporation was filtered and washed in ethanol and dried completely in vacuum. Good single crystals of blue color were obtained from ethanol with a meager amount of water by slow evaporation. The