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Crystallographic Analysis of Coordination Bonding of a Chromium complex with Sulphur Atoms

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Abstract—The complex crystallizes in monoclinic crystal system with space group $P2_1/c$ with unit cell parameters a=12.9923(4)Å, b=21.1463(8)Å, c=18.9922(7)Å, $\beta=93.840(4)$ °, Z=4. The crystal structure was refined to a final reliability index (R-value) of 0.0576 for 5868 observed reflections. The X-ray diffraction analysis reveals a distorted octahedral geometry around the chromium centres. The chromium atom is coordinated by six sulfur atoms from three diphenyldithiophosphato ligands bonded in bidentate chelating fashion. The phosphorus is surrounded by two sulfurs and two oxygen atoms to furnish a distorted tetrahedral geometry. No classic hydrogen bonds are present in complex.

Keywords: Metal complexes, Dithiophosphates, XRD.