Synthesis and Crystal Structure of $[Co(HL)L]\cdot CH_3OH$ (H_2L = Pyridoxal S-methylisothiosemicarbazone)

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Brown single crystals of the title compound, $C_{21}H_{29}CoN_8O_5S_2$, were prepared by the reaction of MeOH solutions of $Co(Oac)_2\cdot 4H_2O$ and $H_2L\cdot H_2O$ in mole ratio 1 : 1. The complex has a *mer*-octahedral configuration with two non-equivalent tridentate ligands with O,N,N donors: one of the ligands having deprotonated isothiosemicarbazido fragment, whereas for the other additional deprotonation involves the pyridine nitrogen. The compound crystallizes in the P $2_1/c$ space group with a = 11.375(3) Å, b = 14.263(5) Å, c = 15.854(6) Å, β = 99.63(2)°, V = 2535.9(15) Å^3. X-ray diffraction data were recorded on an Enraf-Nonius CAD-4 diffractometer with graphite monochromated Mo $K\alpha$ radiation (λ = 0.71069 Å). Anisotropic refinement of all non-hydrogen atoms converged to R = 0.0567 for 4966 independent reflections and 356 parameters.

Keywords: cobalt(III) complex, pyridoxal S-methylisothiosemicarbazone, mer-octahedral configuration