Crystal structure and DFT computational studies on diaquabis (pyridine) cobalt (II) dichloride

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Description
Single-crystal diffraction experiment was carried out using the high-resolution home diffractometer equipped with an area detector. Data sets were collected at room temperature (293 K) Mo K_α radiation (λ = 0.71073 Å). The molecule structure of Diaquabis(pyridine) cobalt(II) dichloride crystallizes in a space group *P-1* of triclinic system with cell parameters a = 6.1718(3) Å, b = 6.5395(3) Å, c = 8.5379(4) Å, á = 109.199(3)°, â = 102.822(3)°, γ = 97.484(3)° and V = 309.49(3) $Å^3$. The molecular geometry were calculated using the density functional method (B3LYP) with 3-21G basis set. The calculated results show that the optimized geometry can well reproduce the crystal structure. The electric dipole moment (μ), the polarizability (α) and the first hyperpolarizability (β) were calculated using the density functional B3LYP method with the lanl2dz basis set. For the results, the title compound shows nonzero (β) value …