Crystal Structure and Conformation of N-(5-Chlorosalicylidene)-2-hydroxy-5-chloroaniline

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N-(5-Chlorosalicylidene)-2-hydroxy-5-chloroaniline was synthesized and its crystal structure determined. It crystallizes in the orthorhombic space group $Pn\alpha_2$ with $a = 14.668(4)$, $b = 6.084(3)$, $c = 27.980(4) \text{Å}$, $R = 0.051$ for 4788 independent reflections). There are two independent nearly planar molecules in the asymmetric unit. The intramolecular hydrogen bonds occur between the pairs of atoms N1 and O1 [2.553(6)Å], N1 and O2 [2.585(5)Å], N2 and O3 [2.567(6)Å], N2 and O4 [2.620(5)Å], the hydrogen atoms essentially being bonded to the nitrogen atoms. The neighboring molecules are linked via an intermolecular O-H...O hydrogen bond [2.557(5)Å]. Conformations of the title compound were investigated by semi-empirical quantum mechanical AM1 calculations. The optimized geometry of the molecular structure corresponding to the nearly planar conformation is the most stable conformation in the calculations. The results strongly indicate that the minimum energy conformation is primarily determined by non-bonded steric interactions.