Investigation of intermolecular interactions in the crystal structure of 1-phenyl-1,2-ethanediol

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Abstract: 1-Phenyl-1,2-ethanediol was synthesized from the hydrolysis of epoxy styrene in water medium. The compound was characterized by FT-IR and NMR spectroscopic methods and structure was characterized by single crystal X-ray diffraction method. The crystallographic information was collected at 293 K. This compound is crystallized in the triclinic P1 space group with unit cell parameters of a = 6.0274(10) Å, b = 16.204(2) Å, c = 17.345(2) Å; α = 117.584(14)°, β = 99.322(13)°, γ = 90.047 (14)°, V = 1476.1 (4) Å3 and Z = 8. The asymmetric unit of the crystal structure consists of four molecules of 1-phenyl-1,2-ethanediol which are connected to each other by strong hydrogen bond and C-H···π interactions. A supramolecular network is generated by intermolecular O-H···O and C-H···O hydrogen bond interactions.

Keywords: 1-Phenyl-1,2-ethanediol; crystal structure; hydrogen bonding.

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