

structure for the same molecule, has been suggested as “an anathema to crystal engineering” [1], and the same might well be said about crystal structure prediction. Polymorphism is of special importance in pharmaceutical industry processes, where different physical properties of polymorphic forms can substantially alter the viability and quality of a product such as drug [2]. Comparisons of the intermolecular interactions in polymorphic structures are very important for elucidating their properties. Hirshfeld surface is becoming a valuable tool for analyzing intermolecular interactions while maintaining whole-of-the size and shape of a Hirshfeld surface reflects the interplay between different atoms and intermolecular contacts in a crystal, and hence the surface necessarily reflect different intermolecular interactions.molecule approach [3]. In this study, we report the crystal structure and Hirshfeld surface analysis of two polymorphs of a potentially bidentate diimine ligand.

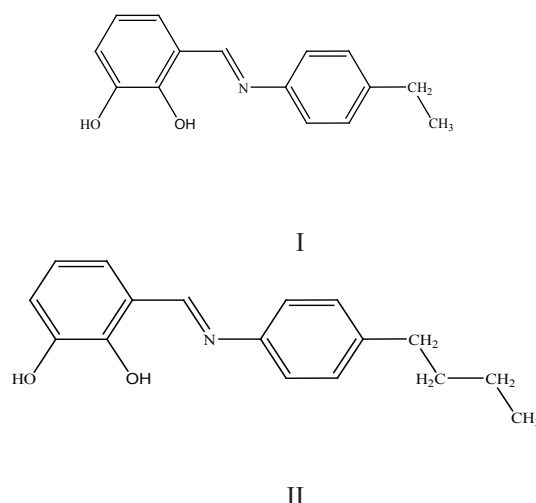
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Keywords: polymorphism; crystal structure; hirshfeld surface

FA4-MS05-P13

Crystal Structure of (E)-3-[(4-Ethylphenylimino)methyl]benzene-1,2-diol and (E)-3-[(4-Butylphenylimino)methyl]benzene-1,2-diol. Zeynep Keleşoğlu^a, Başak Koşar^a, Çiğdem Albayrak^b, Mustafa Odabaşoğlu^c, Orhan Büyükgüngör^a. ^a*Department of Physics, Ondokuz Mayıs University, Samsun, Turkey.* ^b*Faculty of Education, Sinop University, Sinop, Turkey.* ^c*Denizli Technical Vocational School, Pamukkale University, Denizli, Turkey.*
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Schiff bases are widely used as ligands in the field of coordination chemistry and they play an important role in various field of chemistry due to their biological activities [1]. *o*-Hydroxy Schiff bases derived from the reaction of *o*-hydroxy aldehydes with aniline have been examined extensively [2]. Some Schiff bases derived from salicylaldehyde have attracted the interest of chemists and physicists because they show thermochromism and photochromism in the solid state by H-atom transfer from the hydroxy O atom to the N atom [3]. It has been proposed that molecules showing thermochromism are planar while those showing photochromism are non-planar [4]. Here we report the molecular and crystal structure of (E)-3-[(4-Ethylphenylimino)methyl]benzene-1,2-diol, (E)-3-[(4-Butyl phenylimino)methyl]benzene-1,2-diol labeled as I and II, respectively.



The crystal structures were solved by direct methods and refined by full matrix anisotropic least-squares methods. There are two types of intramolecular hydrogen bonds in Schiff bases arising from the keto-amin (N-H...O) and enol-imine (N...H-O) tautomeric forms. X-ray investigation shows that both compound I and II prefer the enol-imine tautomeric form with a strong intramolecular O-H...N hydrogen bond.

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Keywords: schiff bases; enol-imine

FA4-MS05-P14

Crystal Structure of 2-(4-Bromophenylimino)methyl-3,5-dimethoxyphenol. Işın Kiliç^a, Ferda Erşahin^b, Erbil Ağar^b, Şamil Işık^a. ^a*Ondokuzmayıs University, Department of Physics, Samsun- Turkey.* ^b*Ondokuzmayıs University, Department of Chemistry, Samsun- Turkey.*
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The crystal structure of the title compound, C₁₅H₁₄O₃NBr, contains two independent molecules in the asymmetric unit. The two molecules of the asymmetric unit have very similar geometrical parameters and adopt the phenol-imine tautomeric form, with strong intramolecular O—H...N hydrogen bonds. The title compound crystallizes in the monoclinic space group P -1 with the following unit-cell parameters: a = 8.2655(5) Å, b = 9.7305(6) Å, c = 18.3806(11) Å, α = 97.177(5)°, β = 92.796(5)°, γ = 106.214(5)° and V = 1402.94(15) Å³. Both molecules are not planar and the dihedral angles between the two benzene rings are 24.64(0.21) and 30.30(0.13) Å.

Keywords: X-ray crystallography of organic compounds; 5-dimethoxyphenol; 4-Bromophenylimino