

of  $C_{14}H_{12}ClNO$ , was collected with using MoK $\alpha$  radiation in 296 K. Compound was crystallised on orthorhombic system, space group Pbc $a$   $a = 7.5121(7) \text{ \AA}$ ,  $b = 11.9190(15) \text{ \AA}$ ,  $c = 27.500(3) \text{ \AA}$ ,  $V = 2462.3(5) \text{ \AA}^3$ ,  $Z = 8$ .

Data collection and cell refinement: Stoe X-Area. To solve and refine the structure we used the programs SHELXS-97 and SHELXL-97, respectively. Molecular graphics: ORTEP3 for Windows.

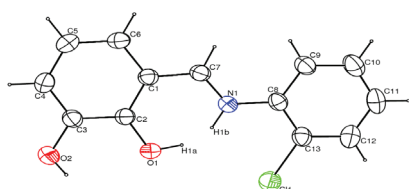
**Keywords:** schiff base; enol-imine; anti-tumour

#### FA4-MS05-P10

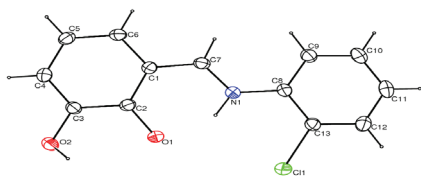
**The Structure of (Z)-6-[(2-chlorophenylamino)methylene]-2-hydroxycyclohexa-2,4-dienone at Two Different Temperatures.** Ersin Temel<sup>a</sup>, Çiğdem Albayrak<sup>b</sup>, Mustafa Odabaşoğlu<sup>c</sup>, Orhan Büyükgüngör<sup>a</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. <sup>b</sup>Sinop Faculty of Education, Sinop University, Sinop, Turkey, <sup>c</sup>Denizli Technical Vocational School, Pamukkale University, Denizli, Turkey.

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The crystal structure of the title compound, a Schiff base, was determined at 296 K and 100 K. The position of hydrogen atom characterizing the Schiff base type could not be certainly determined at 296 K. However, it can be said that the OH form is more dominant than NH form, with the percentages of 58 and 42, respectively. On the other hand, at 100 K it is found that the H atom is bonded to N atom. The packing is mainly stabilized by inter-molecular hydrogen bonds of O-H...O type. These hydrogen bonds give rise to  $R_2^2(10)$  dimeric rings in the extended structure. The packing is also supported by  $\pi \dots \pi$  interactions between benzene rings.



(a) 296 K



(b) 100 K

Fig. Perspective views of title compound with the atom numbering scheme: (a) at 296 K and (b) at 100 K.

**Keywords:** X-ray crystallography; schiff base

#### FA4-MS05-P11

**Crystal Structure and Quantum Mechanical Calculations of (E)-4-methoxy-2-[(o-tolylimino)methyl] phenol.** Arzu Özek<sup>a</sup>, Orhan Büyükgüngör<sup>a</sup>, Çiğdem Albayrak<sup>b</sup>, Mustafa Odabaşoğlu<sup>c</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey. <sup>b</sup>Faculty of Education, Sinop University, Sinop, Turkey. <sup>c</sup>Denizli Technical Vocational School, Pamukkale University, Denizli, Turkey.

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Schiff base ligands are very important compounds in the chemical industry and medicine. In general, O-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and ketoamine (or quinoid) forms. Depending on the tautomers, two types of intramolecular hydrogen bonds are possible: O—H...N in benzenoid and N—H...O in quinoid tautomers. The H atom in title compound (I) is located on atom O1, thus the phenol-imine tautomer is favored over the keto-amine form, as indicated by the C2—O1, C8—N1, C1—C8 and C1—C2 bond lengths. A similar work was also observed in our previous work [1]. In the crystal structure, weak intermolecular C—H...O hydrogen bonds results in the formation of C(5) chains along the c axis, in which they may be effective in the stabilization of the structure.

The experimental geometry of title compound (I) obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations (semi-empirical, ab-initio Hartree-Fock HF and density-functional theory DFT/B3LYP). Ab-initio HF, DFT and semi-empirical (AM1 and PM3) calculations and full-geometry optimizations were performed by means of GAUSSIAN 03W package [2]. We observe an acceptable general agreement between them. Although the DFT molecular orbital theory was considered as the most accurate method for geometry optimization for free and complex ligands [3], the HF method led to better results in regard to the bond lengths and angles.

[1] Özek, A., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2008). J. Chem. Crystallogr. in print. [2] Friesner, R. A. (2005). PNAS 102, 6648. [3] Frisch, M. J. et al. (2004). GAUSSIAN03 Revision E.01. Gaussian, Inc., Wallingford CT 06492, USA.

**Keywords:** single-crystal X-ray diffraction; quantum mechanics

#### FA4-MS05-P12

**Two Monoclinic Polymorphs of Bis(4-cyanobenzylidene)Butanediamine: The Crystal Structure and Hirshfeld Surface Studies.** Reza Kia<sup>a</sup>, Hoong-Kun Fun<sup>a</sup>. <sup>a</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800, Penang, Malaysia.

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Polymorphism, the existence of more than one crystal

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.

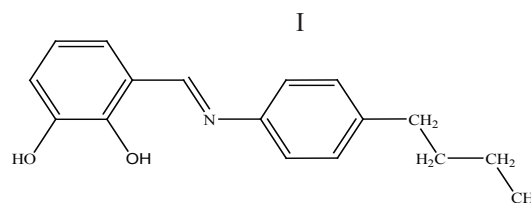
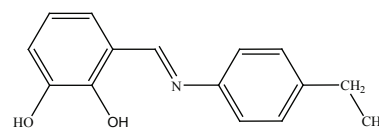
[1] Bernstein, J., Henck, J. *Cryst. Eng.* **1998**, 1, 119. [2] Haleblan, J., McCrone, W. *J. Pharm. Sci.* **1969**, 58, 911. [3] McKinnon, J. J., Jayatilaka, D., Spackman, M. A. *Chem. Commun.*, **2007**, 3814.

**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<sup>a</sup>, Başak Koşar<sup>a</sup>, Çiğdem Albayrak<sup>b</sup>, Mustafa Odabaşoğlu<sup>c</sup>, Orhan Büyükgüngör<sup>a</sup>. <sup>a</sup>Department of Physics, Ondokuz Mayıs University, Samsun, Turkey. <sup>b</sup>Faculty of Education, Sinop University, Sinop, Turkey. <sup>c</sup>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.



II

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.

[1] Lozier, R.; Bogomolni, R. A.; Stoekenius, *W. J. Biophys.* **1975**, 15, 955. [2] Calligaris, M.; Randaccio, L. *Comprehensive Coordination Chemistry*, G. Wilkinson Eds., Pergamon, London **1987**, 715. [3] Hadjoudis, E.; Vitterakis, M.; Mavridis, I. M. *Tetrahedron* **1987**, 43, 1345. [4] Moustakali-Mavridis, I.; Hadjoudis, E.; Mavridis, *A. Acta Cryst.* **1980**, B36, 1126.

**Keywords:** schiff bases; enol-imine

#### FA4-MS05-P14

**Crystal Structure of 2-(4-Bromophenylimino)methyl-3,5-dimethoxyphenol.** İşın Kiliç<sup>a</sup>, Ferda Erşahin<sup>b</sup>, Erbil Ağar<sup>b</sup>, Şamil İşik<sup>a</sup>. <sup>a</sup>Ondokuzmayıs University, Department of Physics, Samsun- Turkey. <sup>b</sup>Ondokuzmayıs University, Department of Chemistry, Samsun- Turkey.  
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The crystal structure of the title compound, C<sub>15</sub>H<sub>14</sub>O<sub>3</sub>NBr, 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)Å<sup>3</sup>. 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