

of $C_{14}H_{12}ClNO$, was collected with using MoK α 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.

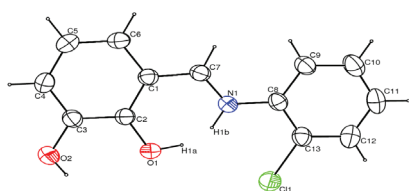
Keywords: schiff base; enol-imine; anti-tumour

FA4-MS05-P10

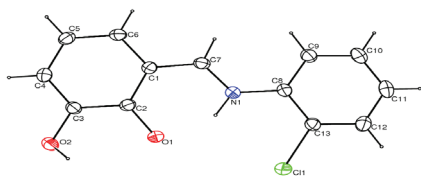
The Structure of (Z)-6-[(2-chlorophenylamino)methylene]-2-hydroxycyclohexa-2,4-dienone at Two Different Temperatures. Ersin Temel^a, Çiğdem Albayrak^b, Mustafa Odabaşoğlu^c, Orhan Büyükgüngör^a. ^aDepartment of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. ^bSinop Faculty of Education, Sinop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

E-mail: etemel@omu.edu.tr

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^a, Orhan Büyükgüngör^a, Çiğdem Albayrak^b, Mustafa Odabaşoğlu^c. ^aDepartment of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey. ^bFaculty of Education, Sinop University, Sinop, Turkey. ^cDenizli Technical Vocational School, Pamukkale University, Denizli, Turkey.

E-mail: arzuozek@omu.edu.tr

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^a, Hoong-Kun Fun^a. ^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800, Penang, Malaysia.

E-mail: zsrkk@yahoo.com

Polymorphism, the existence of more than one crystal