FA4-MS36-P01

Experimental and DFT studies of (E)-1-((3-bromophenylimino)methyl)naphthalene 2-ol. Tufan Akbal[a], Ahmet Erdönmez[a] and Erbil Ağar [b],
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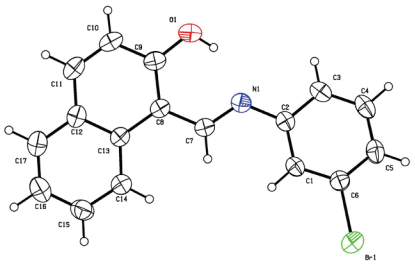
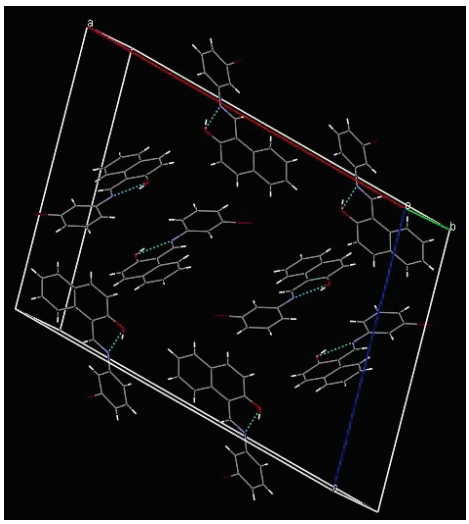
The title compound, $C_{17}H_{12}BrNO$, crystallizes in a enol imine tautomeric form.
The structure is stabilized by O-H…N intramolecular hydrogen bonds. Molecular geometry from X-ray experiment of the title compound in the ground state have been compared using the density functional method (B3LYP) with 6-31G(d,p) basis set. To determine conformational flexibility, molecular energy profile of the title compound was obtained by DFT calculations with respect to two selected degrees of torsional freedom, which were varied from−180º to +180º in steps of 10º. The two rings are not coplanar and dihedral angle them is $16.73(0.17)^0$. The C9-O1 and C7-N1 bond lengths verify the enol-imine tautomeric form. These distances agree with the literature [1]. The C6-Br1 bond length in is also in a good agreement with the corresponding distances in the literature [2].

[1] Karadayi, N., Gözüyesil, S., Güzel, B., Kazak, C. & Büyükgüngör, O. (2003). *Acta Cryst.* E59, o851-o853. [2] Zarife Sibel G., Ağar Alaman A., Işık Ş., (2007). *Acta Cryst.* E63, o4564.

Keywords: tautomerism, crystal and molecular structure, density functional theory(DFT) studies





FA4-MS36-P02

Structural Analysis and DFT calculations of (E)-1-((4-chlorophenylimino)methyl)-napthalen-2-ol. Ahmet Erdönmez[a], Gökhan Alpaslan[a], Mustafa Macit[b], Orhan Büyükgüngör[a], [a]*Ondokuz Mayıs Univ., Department of Physics, Samsun-Turkey,* [b]*Ondokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.*
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The molecular and crystal structure of the title compound, $C_{21}H_{12}ClN_3O$, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group $P2_1/c$ with unit cell dimensions a= 4.7596(2), b= 20.3483(7), c= 14.3293(6), β=82.857(6)°, V= 1330.45(9)Å^3, Z=4, R_1=0.038 and wR_2=0.093.
Crystallographic analysis reveals that the title compound, $C_{17}H_{12}NOCl$, possesses both OH and NH tautomeric character in its molecular structure. The occupancies of the enol and keto tautomers are 0.51(5) and 0.49(5) respectively. In order to explain the tautomerizm process and its effects on the molecular geometry in the solid state, the geometry optimization in gas phase for enol and keto tautomers of the title compound were calculated using density functional method (B3LYP) with the 6-31G(d,p) basis set. To be able to describe the potential barrier height for the intramolecular proton transfer, Potential Energy Surface (PES) scan was performed based on the optimized geometry of enol tautomeric form at the B3LYP/6-31G(d,p) level by varying the redundant internal coordinate O-H bond distance. The calculated results show that the enol form is also predicted to be 1.21 kcal/mol more stable than the keto form in the gas phase by the DFT method.

Keywords: crystal structure analysis, density functional theory, tautomerism

FA4-MS36-P03

Asp214→Ala Mutation Reorganizes the Active Site of *Citrobacter freundii* Tyrosine Phenol-lyase. Dalibor Milić[a], Tatyana V. Demidkina[b], Dubravka Matković-Čalogović[a], Alfred A. Antson[c], [a]*Department of Chemistry, Faculty of Science, University of Zagreb, Croatia,* [b]*Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, Russia,* [c]*York Structural Biology Laboratory, Department of Chemistry, University of York, UK*
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Tyrosine phenol-lyase (TPL) from *Citrobacter freundii* and other bacteria is a homotetrameric protein. This pyridoxal-5'-phosphate (PLP)-dependent enzyme catalyzes the reversible hydrolytic cleavage (β-elimination reaction) of L-tyrosine to give phenol and ammonium pyruvate [1]. The active site (one per each subunit) is situated at an interface between the small and large domain of one subunit, and the large domain of the adjacent subunit [2]. It can assume either the open or closed conformation [3]. We suggest that the active site closure is fundamental to the cleavage of L-tyrosine Cβ–Cγ bond [4]. D214A and D214N TPL mutants from *C. freundii* were shown to be inactive for the β-elimination of L-tyrosine and its derivatives [5]. We present the structure of D214A TPL mutant solved at 1.9 Å resolution. This structure indicates that