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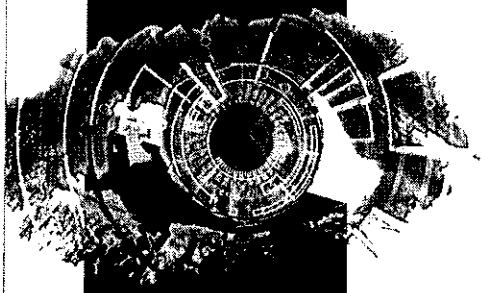

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ABSTRACT BOOK

(Özet Kitapçığı)

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Computational and Structural Analysis of $C_{14}H_{12}BrNO$

Şehriman Atalay[1], Aslı Tosyalı Karadağ[2], , Hakan Bülbül[3], Hasan Genç[4]
[1] *Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, Samsun, Turkey, atalays@omu.edu.tr*
[2] *Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, Samsun, Turkey,* asli.*karadag@omu.edu.tr*
[3] *Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, Samsun, Turkey, hbulbul@omu.edu.tr*
[4] *Yüzüncü Yıl University, Faculty of Arts and Sciences, Department of Chemistry, Van, Turkey h_genc2000@yyu.edu.tr*

Absract

In the title compound, $C_{14}H_{12}BrNO$, is a Schiff base which adopts the phenol–imine tautomeric form in the solid state. The dihedral angle between the two aromatic rings is 34.26 (9)_ and an intramolecular O-H ··· N hydrogen bond generates an S(6) ring. Theoretical calculations using DFT(B3YLP) and HF methods were used to confirm the molecular structure.

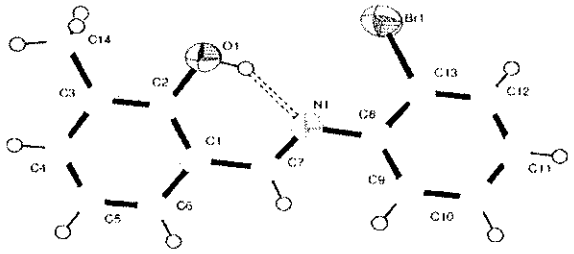

Fig 1 The molecular structure showing 30% probability displacement ellipsoids

Keywords: Single-crystal X-ray study, DFT, HF, Molecular electrostatic potential.