Conformations and Structures of N,N'-Bis(2-methoxybenzylidene)-1,3-diamino-propanol and N,N'-Bis(3-methoxybenzylidene)-1,3-diamino-propanol

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N,N'-bis(2-methoxybenzylidene)-1,3-diamino-propanol ($C_{19}H_{22}N_2O_4$) **1** and N,N'-bis(3-methoxybenzylidene)-1,3-diamino-propanol ($C_{19}H_{22}N_2O_4$) **2** have been investigated by X-ray analysis and AM1 semi-empirical quantum mechanical method. **1** is in the monoclinic space group C2/c with a = 33.694(6), b = 6.735(1), c = 17.681(3) Å, β = 114.72(2)°, V = 3645(1) Å^3, Z = 8, D_c = 1.248 mg cm^{-3} and μ(Mo-K$_\alpha$) = 0.088 mm^{-1}. **2** is in the monoclinic space group C2/c with a = 19.173(4), b = 7.626(2), c = 11.788(2) Å, β = 91.72(2)°, V = 1722.8(6) Å^3, Z = 4, D_c = 1.320 mg cm^{-3} and μ(Mo-K$_\alpha$) = 0.093 mm^{-1}. The crystal structures of **1** and **2** were solved by direct methods and refined to R = 0.053 for **1** and R = 0.041 for **2**. Both molecules are not planar and **2** has twofold axes on C9 atom. Intramolecular hydrogen bonds occur between O1 and N1 [2.541(3) Å] and between O3 and N2 [2.573(4) Å] atoms for **1** and between O1 and N1 [2.631(2) Å] atoms for **2**. The optimized geometries of the crystal structures of **1** and **2** corresponding to non-planar conformation are the most stable conformation in all calculations. The results strongly indicate that the minimum energy conformation is primarily determined by non-bonded hydrogen-hydrogen and hydrogen-carbon repulsions.

Key words: X-Ray, Schiff Base, AM1, Photochromism, Thermochromism